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**The Microstructural Mechanism of Electromigration Failure
in Narrow Interconnects of Al Alloys**

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Ph.D. Dissertation

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by

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ABSTRACT

This thesis reports a study of the mechanism of electromigration failure in Al-2Cu-1Si thin-film conducting lines on Si. Samples were patterned from 0.5 μm thick vapor-deposited films with various mean grain sizes (G), and had lines widths (W) of 1.3, 2, 4 and 6 μm , providing an effective linewidth (W/G) range of approximately from 0.5 to 3. The lines were aged at various conditions to change the Cu-precipitate distribution and were then tested to failure at $T = 225^\circ\text{C}$ and $j = 2.5 \times 10^6 \text{ A/cm}^2$. Some samples were tested over a range of substrate temperatures, current densities and current reversal times. Aging produces an initially dense distribution of metastable θ' (Al_2Cu ; coherent) in the grain interiors, with stable θ (Al_2Cu ; incoherent) at the grain boundaries. The intragranular θ' is gradually absorbed into the grain boundary precipitates, lowering the density of intragranular precipitates. In the wide lines ($W/G > 1$) the mean time to failure increases slowly and monotonically with pre-aging time and current reversal time. The failure mode is the formation and coalescence of voids that form on grain boundaries with an apparent activation energy of 0.65 eV. In the narrow lines ($W/G < 1$), the lines failed by a transgranular-slit mechanism with an activation energy near 0.93 eV, in which voids forms in the bamboo grains that terminate the longest polygranular segments in the line due to accumulation of a supersaturation of vacancies. The distribution of the polygranular segments and the kinetics of failure varies with the linewidths, which provides an explanation for the dependence of failure statistics on line geometry. Failure occurs after Cu has been swept from the grains that fail. Pre-aging the line to create a more stable

distribution of Cu lengthens the time required to sweep Cu from the longest polygranular segment, and significantly increases the time to failure. In the optimum case when the density of intragranular θ -phase precipitates is maximized, the transgranular-slit failure mechanism is suppressed, and the bamboo grain fails by diffuse thinning to rupture. The results from the current reversal test indicate that the time to sweep Cu in the polygranular segments is longer for longer polygranular segments, and have the consequence that the time to first failure in an array of lines is much longer than predicted by a log-normal fit to the distribution of failure times.

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CHAPTER 1

INTRODUCTION

When an electric current flows through a conductor, a migration of atoms occurs. This phenomenon, which is known as electromigration, is a subject of technological interest primarily in integrated circuit device technology. In the present VLSI technology, aluminum thin films are used as interconnect material because of their various advantageous properties. However, these aluminum interconnects carry current densities greater than 10^5 A/cm^2 and are liable to failure through electromigration. With the continuous demand for advanced device technology in which the reduction of interconnect dimension is essential, the problem of electromigration is becoming a greater limiting factor.

Ever since it was found that electromigration in aluminum interconnects is one of the major sources of device failures, various studies have been done to resolve the problem [1, 2]. These studies revealed that the microstructure of the thin film, combined with the physical parameters of the interconnect such as film thickness, line length and width, play an important role in the electromigration failure. Although these studies established many scientific insights into the failure mechanism, there are many elements that are still unclear. Detailed analysis of the interaction between the failure mechanism and the microstructural factors of thin films is essential in order to provide guidance for the development of reliable interconnects that are suitable for advanced applications.

In this study, the microstructural mechanisms of electromigration failure of Al interconnects were investigated. The focus was the influence of alloying element on the failure mechanism in interconnects with narrow linewidth. This study identifies the failure mechanism of interconnects and its dependence on alloying elements. With this un-

derstanding, several ways to improve the reliability of aluminum interconnects are suggested.

In this chapter, the description of electromigration and its application to Al thin films are introduced to provide a basis for the study. Efforts has been made to summarize the general observations of electromigration failure associated with the microstructure of thin films. The known mechanisms, including diffusional and statistical mechanisms, are briefly discussed.

1.1. Phenomenological description of electromigration

Since electromigration is basically the diffusion of atoms under an external driving force, the irreversible thermodynamics of diffusion can provide a phenomenological description of electromigration [3, 4]. In a multi-component system, the atomic motion of the i^{th} component depends on its interaction with all the other elements in the system. This can be expressed by writing the atomic flux J_i as

$$J_i = \sum_{j=1} L_{ij} X_j \quad (i = 1, 2, \dots, n) \quad (1.1)$$

where L_{ij} is the phenomenological coefficient correlating the flux of the i^{th} component to the driving force X_j of the j^{th} component. In an electric field, the driving force is derived from the gradient of chemical potential μ_i as well as macroscopic electrical potential Φ .

Separating the motion of atoms and charge carriers, eq. (1.1) becomes

$$J_i = -(\sum_j L_{ij} \nabla \tilde{\mu}_j + L_{ie} \nabla \tilde{\mu}_e) \quad (1.2)$$

$$J_e = -(\sum_j L_{ej} \nabla \tilde{\mu}_j + L_{ee} \nabla \tilde{\mu}_e) \quad (1.3)$$

where $\tilde{\mu}_j$ are generalized potentials defined by $\tilde{\mu}_j = \mu_j + Z_j e \Phi$. Here, Z_j represents the ionic valence of the specific atom; it is -1 for free electrons. It can be seen that all diagonal elements of L_{ij} relate to the diffusion coefficients of the i^{th} component, except for

L_{ee} which governs the conductivity of electrons. The off-diagonal elements L_{ij} give the correlation effects on the atomic jumps of the i^{th} element due to the jumps of the j^{th} element, while L_{ie} is related to the interaction between the ion and electrons.

1.1.1. Driving force

In a one component system, the chemical potential gradient of atoms and electrons vanishes, and eqs. (1.2), therefore, can be simplified as

$$J_i = L_{ii}(Z_i - \frac{L_{ie}}{L_{ii}})eE \quad (1.4)$$

where E represents an electric field which has the physical meaning of the gradient of electric potential, $E = -\nabla\Phi$. From this relation, the driving force for electromigration can be obtained:

$$F = (Z - \frac{L_{ie}}{L_{ii}})eE \quad (1.5)$$

where Z denotes the valence of the atom. It can be seen that electromigration results from the two competitive forces: the electrostatic force (ZeE) and the force from the dynamic interaction between moving electrons and atoms ($-L_{ie}/L_{ii} eE$). The latter force is often called "electron wind" or "electron friction" force [5-12]. The physical source of "electron friction force" can be found in the recent review paper by Sorbello [13]. Conventionally, eq. (1.5) is expressed as

$$F = Z^*eE \quad (1.6)$$

where Z^* denotes the effective valence of the metal ion:

$$Z^* = Z - L_{ie}/L_{ii} \quad (1.7)$$

Experimentally measured values of Z^* for various metals are usually negative and large in magnitude. For example, the effective valences of Al, Au and Cu are about -30, -8 and -5, respectively. This result indicates that the electron wind force is usually dominant.

From eqs. (1.4)-(1.7) and Ohm's law, $j = E / \rho$, the electromigration flux becomes

$$J_i = L_{ii} Z^* e E = L_{ii} Z^* e \rho_i j \quad (1.8)$$

where ρ_i and j denote the electrical resistivity of the metal and the applied current density, respectively. Since the diagonal coefficient L_{ii} is the mobility of a pure metal, the Nernst-Einstein definition of mobility, $L_{ii} = C_i D_i / kT$, leads to the full expression of the electromigration flux as

$$J_i = \frac{C_i D_i}{kT} Z^* e \rho_i j \quad (1.9)$$

where C_i and D_i present the concentration and the diffusivity of the metal, respectively. Hence, the electromigration flux of a pure metal is determined by the diffusivity (mobility) and the effective charge Z^* (driving force). When these two factors are compared for pure elements like Au, Cu and Al, the electromigration flux in Al is expected to be more extensive than for the other metals. This is because the diffusivity of Al is much faster, and the effective charge is much higher than other elements. Therefore, electromigration causes Al interconnects to be unreliable in microelectronics devices because it induces damages and failures.

1.1.2. Electromigration in a dilute alloy

The atomic flux of the i^{th} component in a multi-component system is influenced by the j^{th} component as described in eq. (1.1) and (1.2). At this point, not all of the non-diagonal coefficients are independent so that the Onsager's relation cannot be applied to reduce the number of independent coefficients. However, applying the mass conservation condition, i.e.

$$\sum_i J_i = 0 \quad (1.10)$$

and the mechanical equilibrium condition, i.e.

$$\nabla \sum_j \tilde{\mu}_j = 0 \quad (1.11)$$

the reduction of the number of independent L_{ij} can be achieved [14]. For a system in which diffusion takes place through vacancies, it is convenient to introduce the vacancy as an additional component to balance the mass transport of the moving atoms as

$$J_v = -\sum_i J_i \quad (1.12)$$

Adapting lattice reference frame where the atomic motion can be observed from the relative movement of the lattice, the Onsager relation can be applied to yield $L_{ij} = L_{ji}$.

From eq. (1.2) and eqs. (1.10)-(1.12), the mass flux equations for dilute of alloys of solute a and solvent b become

$$J_a = -[L_{aa}\nabla(\tilde{\mu}_a - \nabla\tilde{\mu}_v) + L_{ab}\nabla(\tilde{\mu}_b - \nabla\tilde{\mu}_v)] + L_{ae}\nabla\tilde{\mu}_e \quad (1.13a)$$

$$J_b = -[L_{ba}\nabla(\tilde{\mu}_a - \nabla\tilde{\mu}_v) + L_{bb}\nabla(\tilde{\mu}_b - \nabla\tilde{\mu}_v)] + L_{be}\nabla\tilde{\mu}_e \quad (1.13b)$$

$$J_a + J_b + J_v = 0 \quad (1.13c)$$

In an homogeneous alloy, the chemical potential gradients of the components vanish and eqs. (1.13) become:

$$J_a = (L_{aa}Z_a + L_{ab}Z_b - L_{ae})eE \quad (1.14a)$$

$$J_b = (L_{ba}Z_a + L_{bb}Z_b - L_{be})eE \quad (1.14b)$$

One the other hand, the cross-coefficients L_{ae} and L_{be} , which originate from the interaction of atoms a and b , respectively, with the electrons, are related to the wind forces $Z_a eE$ and $Z_b eE$ by the following relations [14, 15]:

$$\begin{aligned} L_{ae} &= L_{aa}Z_a + L_{ab}Z_b \\ L_{be} &= L_{ba}Z_a + L_{bb}Z_b \end{aligned} \quad (1.15)$$

Hence:

$$\begin{aligned} J_a &= (L_{aa}Z_a^* + L_{ab}Z_b^*)eE \\ J_b &= (L_{ba}Z_a^* + L_{bb}Z_b^*)eE \end{aligned} \quad (1.16)$$

It can be seen that there are additional contributions to the flux of a particular component through coefficient L_{ab} . This cross-term effect on the electromigration is called the "vacancy-flow" effect. This term indicates that there is extra mass flow of b atoms, for example, caused by vacancies pushed to them in an opposite direction as a result of the a atoms.

For dilute alloys, the kinetic analysis of Manning [16] shows that

$$\begin{aligned} L_{aa} &\approx \frac{C_a D_a}{kT} \\ L_{bb} &\approx \frac{C_b D_b f_b}{kT} \end{aligned} \quad (1.17)$$

where D_a and D_b are the uncorrelated diffusion coefficients of the solvent and solute atoms, respectively, and f_b is the solute correlation factor. C_a and C_b represent the concentration of solvent and solute atoms respectively. Using this expression, the atomic flux of solvent and solute atoms can be expressed as

$$\begin{aligned} J_a &= \frac{C_a D_a}{kT} Z_a^{**} eE \\ J_b &= \frac{C_b D_b f_b}{kT} Z_b^{**} eE \end{aligned} \quad (1.18)$$

Here, Z_a^{**} and Z_b^{**} , called the apparent effective charges, are experimentally measured parameters and can be related to the actual effective charges by the following relationships:

$$\begin{aligned} Z_a^{**} &= Z_a^* \left(1 + \frac{L_{ab} Z_b^*}{L_{aa} Z_a^*} \right) \\ Z_b^{**} &= Z_b^* \left(1 + \frac{L_{ba} Z_a^*}{L_{bb} Z_b^*} \right) \end{aligned} \quad (1.19)$$

From the above derivation, one fact becomes clear that the electromigration of solvent atoms is influenced by the apparent effective charge Z_a^{**} through contributions from "vacancy-flow effect". Using eq. (1.17), one can show that

$$\frac{L_{ab}}{L_{aa}} = \frac{D_b^*}{D_a} \frac{L_{ab}}{L_{bb}} C_b \quad (1.20)$$

where $D_b^* = D_b f_b$. Thus, the vacancy-flow correction is linearly proportional to the solute concentration. For most substitutional alloys the sign of Z_b^* is the same as Z_a^* ; so, whether the vacancy-flow effect would increase or decrease the apparent effective charge depends on the sign of L_{ab}/L_{bb} . Also, the contribution is a linear function of the solute concentration. Note that the vacancy-flow effect has the same direction for both the solute and solvent electromigration. For example, if the electromigration of the solvent is enhanced by the presence of solute, the same effect appears in the electromigration of solute.

However, there is another factor to consider other than the vacancy-flow effect in order to evaluate the solute effect; the diffusivity of solvent atoms is influenced by the solute atoms [17, 18]. For dilute alloys

$$D_a = D_a(0)(1 + b' C_b) \quad (1.21)$$

where $D_a(0)$ is the uncorrelated diffusivity of the pure solvent and b' is a constant.

Combining eqs. (1.18)-(1.21), one obtains

$$\begin{aligned} J_a &= \frac{C_a D_a(0) Z_a^* e E}{kT} \left[1 + \left(b' + \frac{D_b^*}{D_a(0)} \frac{L_{ab}}{L_{bb}} \frac{Z_b^*}{Z_a^*} \right) C_b \right] \\ J_b &= \frac{C_b D_b^* Z_b^* e E}{kT} \left(1 + \frac{L_{ab}}{L_{bb}} \frac{Z_a^*}{Z_b^*} \right) \end{aligned} \quad (1.22)$$

Now, the electromigration flux with and without solute can be compared:

$$\begin{aligned} \frac{J_a}{J_a(0)} &= 1 + \alpha_a C_b ; \quad \alpha_a = \left(b' + \frac{D_b^*}{D_a(0)} \frac{L_{ab}}{L_{bb}} \frac{Z_b^*}{Z_a^*} \right) C_b \\ \frac{J_b}{J_a(0)} &= \alpha_b = \frac{D_b^*}{D_a(0)} \left(\frac{L_{ab}}{L_{bb}} + \frac{Z_a^*}{Z_b^*} \right) \end{aligned} \quad (1.23)$$

where α_a and α_b represent the enhancement factor of solvent and solute electromigration, respectively.

Ho [19] estimated the enhancement factors for dilute alloys of Al, Cu, Ag and Au and the results are shown Table 1.1. The results show interesting general features about solute effect on electromigration. First, a vacancy-flow effect would decrease the electromigration of solute and solvent as can be seen from the negative values of L_{ab}/L_{bb} . However, the magnitude of vacancy-flow effect on the electromigration flux of solvent is small and overwhelmed by the diffusivity enhancement effect (b'). Thus, the presence of the solute enhances the electromigration of solvent except for Fe in Cu or Ag.

Table 1.1 Estimation of flux enhancement factors in various alloys.

Solvent	Solute	Z_b^*	Z_b^*/Z_a^*	L_{ab}/L_{bb}	α_b	b'	α_a	α_v
Al	Cu	-6.8	0.4	-0.4	~0	~100	~100	~100
	Zn	-33.9	2.0	-0.79	2.4	19.5	16.3	17.7
	Mg	-52.4	3.1	-0.79	8.3	23.0	14.2	21.5
Cu	Zn	-23.3	2.9	-0.29	7.3	8.4	6.1	12.4
	Fe	-61.3	7.7	-1.2	5.4	-1.2	-8.9	-4.5
Ag	Cu	-16.1	1.3	-0.65	0.56	9.8	9.1	8.7
	Zn	-27.6	2.2	-0.53	4.9	13.5	10.1	14.0
	Cd	-29.1	2.3	-0.73	4.5	11.4	6.5	10.0
	In	-48.9	3.9	-0.71	13.2	17.5	6.0	18.2
	Sb	-115.0	9.2	-1.2	47.5	73.1	7.5	54.0
	Fe	-58.0	4.6	-0.44	2.2	-12.6	-13.7	-12.5
Au	In	-22.2	2.4	-1.3	7.7	84.4	62.5	69.2
	Sn	-32.6	4.5	-1.4	25.9	162.3	101.8	126.7

One significant conclusion obtained from this analysis is that the addition of most solutes to these metals will not reduce the overall rate of electromigration. For example,

the addition of Cu to Al would increase the electromigration rate of Al atoms considerably because of large positive α_a but Cu would migrate little itself ($\alpha_b \sim 0$). This is a somewhat surprising result. Both results disagree with the observations made in several studies in thin films. It has been convincingly shown that the Cu retards the Al electromigration significantly, while Cu itself migrate considerably along the electron flow direction [12-23]. As a result, failure by electromigration in Al thin films is several orders slower than in pure Al, which is the reason why Al interconnects are commonly alloyed with Cu [24]. The same effect was reported in the case of Mg addition to Al thin films [25]. To account for this, several theories have been proposed as will be discussed further in this chapter; however, the answer is still unknown. This question is one of the main points on which this thesis is focused.

1.2 Electromigration in thin films

Electromigration in polycrystalline thin films is different from that in the bulk due to the presence of an unusually high grain boundary density. Since the grain boundary provides an easy path for atom migration, electromigration through grain boundaries is predominant. Defining the grain boundary density as

$$d = \frac{\delta}{G} \quad (1.24)$$

where δ and G represent the thickness of the grain boundary and the mean grain size of the film, respectively, the electromigration flux in a thin film becomes

$$J_g = \frac{C_{gb} D_{gb} d}{kT} \rho_{gb} Z_{gb}^* e j \quad (1.25)$$

where the subscript gb represents the grain boundary [26-28]. Eq. (1.25) is often used without the d factor for simplicity. Several studies, in which activation energy of electromigration flux is studied, confirmed that the electromigration mainly occurs via grain boundaries; the activation energy ranges from 0.35 to 0.7 eV [29-34], which is about a

half of that for lattice diffusion for Al, 1.33~1.48 eV [35-38]. The effective charge in the grain boundary is expected to be different from that in lattice. Although there have been several studies to identify the effective charge in the grain boundary, the reported values are not consistent: they vary from -1 to -10 [39-40].

1.3 Electromigration induced stress in thin films

Stress can be induced as a result of electromigration. Blech and others performed drift velocity measurements, as illustrated in Fig. 1.1, by fabricating a test strip with a controlled length, sitting on a underlayer that has relatively high electrical resistance, such as TiN or Mo [40-43]. When a voltage is applied, the current predominantly flows through the test strip because of its low resistance. Because of electromigration, the material is depleted from one end of the strip and accumulated on the other. The drift velocity of the stripe end provides a measure of the mass transport.

Fig. 1.1 Schematic illustration of test strip that is used to measure the drift velocity of metal ions under the electric current

A typical result of the drift velocity measurement as tested on Au thin films is shown in Fig. 1.2 [41]. It can be seen that strip end moves only when the current density exceeds a threshold value. It is also observed that the end flows backward when the current is removed. The same trend is found in thin films of Al and Al alloys. These results

Fig. 1.2 The measured drift velocity as a function of the current density at 430°C for Au thin films.

Fig. 1.3 The temperature dependence of the current-stripe length product measured in pure Al. The product linearly decreases with increasing temperature.

are attributed to the presence of a stress gradient that is induced as a result of the mass accumulation (compressive stress) and mass depletion (tensile stress) at the ends of the sample. The threshold current density corresponds to the minimum driving force to overcome the effect of the stress gradient. In a steady state, the drift velocity of the strip end can be expressed as

$$v_d = \frac{D_{gb}}{kT} (\rho_{gb} Z_{gb}^* e j - \frac{\Omega \Delta \sigma}{l}) \quad (1.26)$$

where Ω , $\Delta \sigma$ and l represent the atomic volume and the stress difference along the length of strip, l . The threshold current density j_c , is given by

$$j_c = \frac{\Omega \Delta \sigma}{\rho_{gb} Z_{gb}^* e l} \quad (1.27)$$

There also exists threshold strip length l_c under which no strip displacement can occur at a given current density, which can be expressed in the similar form as eq. (1.27) but exchanging l and j . Then, a simple relation between current density and strip length holds:

$$j l_c = j_c l = \frac{\Omega \Delta \sigma}{\rho_{gb} Z_{gb}^* e} = \text{const.} \quad (1.28)$$

The product $j_c l$ or $j l_c$ changes with temperature mainly because of the temperature dependence of the yield strength of the film which limits the amount of the induced stress; the product $(j l)$ estimated in pure Al by Blech is shown in Fig. 1.3 [44]. The threshold strip length l_c , or so called Blech's length, has been measured for pure Al and is on the order of tens of microns for grain sizes on the order of microns. For relatively long strips that terminate in large metal pads, an influence from the electromigration induced stress is expected to be insignificant, which is the usual case for the interconnects in service and in reliability test apparatus.

1.4 Electromigration failure in Al thin films

Extensive amount of electromigration in thin films can cause damage, since a net mass flux is constantly driven from different points in the lines. If electromigration is uniform, as seen in the strip drift test, it is expected that the one end of line is thinned due to the mass depletion, while the other end of the line becomes thicker. However, it was found that the failure in Al thin films is not due to the uniform thinning of the line but to localized void formation. *In situ* TEM study on the electromigration failure morphology showed that voids form at the triple junctions of grains and link with each other along the grain boundaries, resulting in an open circuit [45]. Also, formation of hillocks was found along grain boundaries, which can be an another source of device failure because they can cause a short circuit in the multi-level interconnection [46, 47].

1.4.1 Flux divergence, and void formation and growth

Electromigration flux along the grain boundary can not be uniform because of the flux divergence existing in a thin film microstructure. A simple example of the flux divergence in thin films can be understood using triple points of grain boundary junctions as shown in Fig. 1.4. Assuming that the grain boundary diffusivity is the same for grain boundaries 1, 2 and 3, the electromigration fluxes J_1 , J_2 and J_3 can be represented as

$$\begin{aligned} J_1 &= \frac{C_{gb} D_{gb}}{kT} \rho_{gb} Z_{gb}^* e j \\ J_2 &= J_1 \cos \theta_{12} \\ J_3 &= J_1 \cos \theta_{13} \end{aligned} \quad (1.29)$$

Then the flux divergence

$$\nabla J = J_1 - (J_2 + J_3) \quad (1.30)$$

becomes dependent on the angles θ_{12} and θ_{13} . When $\theta_{12} = \theta_{23} = 60^\circ$, there is no divergence of the flux because incoming flux is balanced with the out-going flux. If, however,

θ_{12} and θ_{23} is less than 60° , out-going flux exceeds the incoming flux ($\nabla J < 0$), and mass is depleted at a triple point. On the other hand, when θ_{12} and θ_{13} are larger than 60° ($\nabla J > 0$), mass is accumulated at the point.

Fig. 1.4 An illustration of the electromigration flux at a triple point of a grain junction.

The void formation mechanism can be described from the mass depletion at the flux divergence point. Since diffusion in Al occurs by the vacancy mechanism, it is convenient to express the electromigration flux in terms of the vacancy flux opposite to the direction of atom flux. The total flux, J_v , is the sum of the drift flux due to electromigration and the diffusive flux due to a concentration gradient developing during the electromigration [48]:

$$J_v = -D \frac{dC_v}{dx} + v_d C_v \quad (1.31)$$

where C_v represents the vacancy concentration and the drift velocity has the same form as eq. (1.26). Then, when the supersaturated vacancies at flux divergence reach the critical concentration, voids form, and the diffusion equation becomes

$$\frac{dC_v}{dt} = -\Delta J_v + \frac{C_v - C_o}{\tau} \quad (1.32)$$

in which C_o and τ are the equilibrium vacancy concentration and the average lifetime of vacancies, respectively.

Although the triple points of grain junctions appear to be the most favorable sites for the initiation of voids because of the large flux divergence associated with them, it should be noted that the overall distribution of these triple points is important for the growth of the voids. Hence, the time and the location for the failure are basically the result of a statistical process, depending on the spatial distribution of flux divergent sites.

Fig. 1.5 Flux divergence induced by the temperature gradient across the line under high current density.

Besides the grain structure of thin films, there are many other potential sources that can result in flux divergence. A temperature gradient imposed on the interconnect is a typical example of a source of flux divergence. In the usual case, the temperature is not uniform along the interconnect [2, 49]. The temperature at the current pad is lower than the interconnect due to a lower current density, and, therefore, acts as heat sink. As a result, a temperature gradient is induced along the line as schematically shown in Fig. 1.5. Since electromigration flux is determined by the temperature at a given current density, flux divergence appears. Thermo-migration would also cause the divergence. In this

case the failure usually appears at the anode end of interconnects. Any structural, thermal and physical property inhomogeneity in interconnects contributes to the flux divergence.

1.4.2 The time to failure and its distribution.

Due to electromigration, the interconnects in microelectronics devices are liable to fail during service, which may limit the expected lifetimes of the devices. Thus, it is essential to estimate the reliability of interconnects under electromigration and then find various ways to control the problem. Since actual microelectronic devices contain thousands of interconnects, it is not practical to test all of these interconnects. Instead, the electromigration failure is simulated by fabricating test units that contain a similar interconnect structure to the actual device. Then, these units are tested under controlled conditions which accelerate the failure and allow the tests to be completed in a reasonable amount of time.

Fig. 1.6 The estimation of reliability margin by extrapolating the lifetime distribution on log-normal probability paper.

In order to obtain the proper statistical distribution of the time to failure, it is necessary to test at least 8 lines [50], although more tests will certainly provide a more accurate evaluation of the distribution. The distribution of time to failure is then characterized by two statistical factors: median time to failure (MTF) and deviation of time to failure (DTF). Since it is known that the time to failure of interconnects follow a log-normal distribution [51-53], it is conventional to fit the distribution of the time to failure to a log-normal distribution. The reliability of the interconnects in the actual device can be extrapolated from the MTF and DTF. Since the first failure limits the reliability of the device, the margin of the reliability is normally set to the initial 0.01% to 0.1% of the failures [54]. This reliability estimation process is schematically illustrated in Fig. 1.6, which shows the distribution of time to failure as a function of cumulative probability.

There are two more factors to be considered in order to complete the evaluation of reliability: activation energy and current exponent. Since electromigration tests are usually performed under accelerated conditions that involve higher current densities and temperatures than the actual service conditions, the activation energy that governs lifetime and the current exponent must be available to extrapolate the data. Black [55] proposed an empirical equation to describe the MTF variation of the form

$$MTF = A j^{-n} \exp\left(\frac{E_a}{kT}\right) \quad (1.33)$$

where A , E_a and n donate a constant, apparent activation energy and current exponent. Ideally, the MTF should be inversely proportional to the electromigration rate or drift velocity as defined in eq. (1.26). In this case, E_a is the same as the activation energy of grain boundary diffusivity, and n is 1. While it was found that the activation energy is similar to that of the grain boundary diffusion [31-34], the current exponent is not found to be 1 but usually greater than 2 [56-58]. Theoretical work done by Shatzkes and Lloyd [59], in which the accumulation of vacancies is calculated in a grain boundary during electromigration, suggest that the exponent could be 2 in an ideal case. A current expo-

ment greater than 2 is often attributed to the effect from Joule heating that changes the temperature of lines during testing [56, 57]. However, the current exponent is still controversial due to the limited amount of both experimental and theoretical work.

Care must be taken when eq. (1.33) is used to extrapolate the reliability of interconnects because the DTF may not be a constant. Bobbio and Saracco and Lloyd pointed out that DTF can vary due to variations in the thermal characteristics and testing conditions of the lines [60, 61]. Also, Joule heating can significantly change DTF and the current exponent [62].

1.5. Electromigration failure and microstructure of Al and Al alloys

The statistical nature of electromigration failures imposes a great deal of complication on the analysis of the failure mechanism. The grain size, grain size distribution and preferred orientation of films can change the overall behavior of electromigration failure. However, even for a given microstructure, the physical parameters of the interconnects such as the linewidth and length are found to be more important because they change the statistical arrangement of grains in thin films. The MTF and DTF vary with such parameters and the variation sheds some lights on the failure mechanism. Also, it was found that alloying elements influence the mechanism, presumably due to their interaction with the grain boundary electromigration. All of these factors and the corresponding effects are summarized in the following sections.

1.5.1 Effect of intrinsic microstructure

Electromigration in thin films occurs mainly through the grain boundaries. Hence, a reduction in grain boundary electromigration can enhance the resistance against failure. The amount of electromigration flux can be simply reduced by making the grain size larger and with a preferred orientation. While a larger grain size reduces the grain

boundary density in thin films, the preferred orientation reduces the grain boundary diffusion. Either one of these modification can increase the electromigration lifetime because they reduce the electromigration flux.

The distribution of grain size also has a great influence on the lifetime because of its effect on the flux divergence. A thin film of perfectly uniform grain size would not exhibit any void formation because there is no flux divergence along the line; an equilibrium or uniform grain structure provides grain junctions with 120° angle in which incoming flux and out-going flux is balanced. As grain size deviates from the ideal case, there should be grain junctions in which the flux diverges and failure occurs. TEM studies on the failure sites showed that the failure occurs at the points where the grain size is abruptly changed, which is a result of distribution of grain size in thin films [34].

Experimentally, Vaidya and Sinha [63] examined the contribution of the above three microstructural factors to the electromigration lifetime and showed that the MTF is proportional to a single microstructure parameter, η , containing the average grain size (G), the variation of grain size (σ_g) and the degree of preferred orientations of the grains:

$$MTF \propto \eta = \left(\frac{G}{\sigma_g^2}\right) \log(I_{111} / I_{200})^3 \quad (1.34)$$

where the degree of preferred orientation was measured from the x-ray diffraction intensity of (111) and (200) planes.

1.5.2 The effect of linewidth

A number of studies have been shown that MTF and DTF depend strongly on the linewidth (W) for a given microstructure [64-67]. It was found that there is a critical linewidth below which electromigration lifetime dramatically changes. When the linewidth is larger than the critical linewidth, MTF increases linearly with linewidth, while DTF decreases linearly. On the other hand, both MTF and DTF exponentially increase with a decrease of linewidth below the critical linewidth. It was found that the

critical linewidth appears when the linewidth is comparable to the mean grain size (G) of the film. By introducing effective linewidth W/G , the linewidth dependence of electromigration lifetime is schematically illustrated in Fig. 1.7.

As shown in Fig. 1.8, as linewidth decreases, the line contains more bamboo grains, i.e. grains which span the entire linewidth. Provided that the electromigration is from left to right, the probable failure site would be the site where the maximum flux divergence occurs, as noted with dashed lines. The failure site in wide lines is determined by the overall connections of grains. On the other hand, the failure site in a near-bamboo structure is strongly dependent on the local arrangement of grains. As can be seen in the figure, near-bamboo structures contain occasional polygranular segments which are bracketed by bamboo grains. These polygranular segments are the most probable sites for the failure and the flux divergence condition at these segments should determine the lifetime to failure. In the extreme case, there is no polygranular portion of line; this is called a hyper-bamboo structure. In this case, electromigration is not carried by the grain boundaries but by the lattice, for there is no continuous grain boundary for electromigration. Several models and simulations have been introduced to demonstrate the lifetime variation with linewidth in terms of grain structure change in lines and they can be categorized into two groups: physical models [68-72] and statistical models [67, 73-75].

1.5.2.1 Physical model

The electromigration flux in a near-bamboo structure is confined to the polygranular segments. In this case, the situation of electromigration in the segment is similar to the experiment of the drift velocity measurement introduced in section 1.3. The length of the polygranular segment is comparable to the test strip length l , and the drift velocity of electromigration in the segment can be the same as eq. (1.26). Combining eq. (1.26) with eq. (1.28), the drift velocity in the segment can be expressed in terms of Blech length and the segment length:

Fig. 1.7 The dependence of MTF and DTF on the effective linewidth.

Fig. 1.8 An example of grain structure variation with effective linewidth. (a) Wide lines contain several grains across the width, while (b) narrow lines have a near-bamboo structure with occasional polygranular segments. (c) When the effective width is extremely small, the line consists of single grains with no polygranular segments.

$$v_d = v_d^* \left(1 - \frac{l_c}{l}\right) \quad (1.35)$$

where v_d^* represents the drift velocity of electromigration without influence from stress gradient, or drift velocity as $l \rightarrow \infty$. Eq. (1.35) indicates that the electromigration flux decreases as the segment length decreases; it takes longer time to fail the shorter segment length. As the linewidth decreases in a near-bamboo structure, the poly-granular segment length also decreases, resulting a in rapid increase in MTF . This model provides qualitative explanations for the experimental observations. However, this model can not provide a feasible explanation for the DTF change. In terms of reliability, DTF is the more important factor to consider.

1.5.2.2. Statistical model

The statistical model for the linewidth dependence of electromigration lifetime was first explored by Agarwala *et al.* [73] and followed by various others [67, 74, 75]. This model assumes that there exist potential failure sites or "failure units" in the thin film microstructure such as triple points of grain junctions. The time to failure of each individual failure unit depends on the flux divergence under electromigration and then, the time to failure of each individual unit, $f(t)$, can be assumed to be distributed log-normally. When lines are patterned out of this microstructure to have a certain length, the number and arrangement of failure units must scale with the linewidth.

In wide lines, several failure units are connected across the width, and failure occurs when these failure units are linked together. Hence, the failure units in wide lines can be modeled as series of links in which failure units are connected in parallel. On the other hand, failure units in near bamboo grains can be modeled as a serial connection of failure units. The concept of serial and series of parallel connection is presented in Fig. 1.9 [67]. In the series of parallel connection, failure occurs at the weakest link, and

then the lifetime is mainly determined by the strongest unit in the weakest link. Similarly, in serial connection, failure occurs at the weakest unit, which determines the lifetime.

Fig. 1.9 Statistical arrangement of failure units in wide lines (a) and narrow lines (b).

When the probability of the failure of any individual unit in time t is

$$F(t) = \int_0^t f(t) dt \quad (1.36)$$

where $f(t)$ is the distribution function of failure unit lifetime, then for a units in parallel, the probability of failure of the lines, $G_p(t)$, is given by

$$G_p(t) = [F(t)]^{N_p} \quad (1.37)$$

where N_p is the number of parallel units (n^{th} order statistics). Eq. (1.37) physically represents the probability to choose the strongest failure units (maximum extreme). For units in series, the probability of failure of the lines is determined by the weakest units (1st order statistics: minimum extreme) and is given by

$$G_s(t) = 1 - [1 - F(t)]^{N_s} \quad (1.38)$$

where N_s is the number of serial failure units. For a wide lines, failure units are in the series of parallel connections (Fig. 1.9.a), and, therefore, the probability of failure $G_{sp}(t)$ can be expressed as

$$G_{sp}(t) = 1 - [1 - F(t)^{N_p}]^{N_s} \quad (1.39)$$

Now, as linewidth increases in wide lines, the number of failure units in parallel connection, N_p , increases because lines contain more grains, and, accordingly, the probability to contain stronger failure units increases and becomes more uniform. Hence, MTF increases, while DTF decreases with linewidth. On the other hand, for a near bamboo structure, the number of failure units, N_s , rapidly decreases with decreasing linewidth. Agarwala and Attardo [73] showed that MTF and DTF obtained from eqs. (1.38)-(1.39) increases exponentially as N_s decreases.

The statistical model is fundamentally different from the physical model in terms of reliability issues. According to the physical model, the reliability of narrow interconnects will be actually improved by decreasing the effective linewidth by making polygranular segments shorter. However, according to statistical model, the low percent failure times cannot be changed with the variation of effective linewidth because the statistical model describes the MTF and DTF variation in terms of scaling of failure units from a fixed distribution. The lifetime of the low percent failures or the very first failure is the always the same for any effective linewidth. This shortcoming of the statistical model stems from the assumption that the distribution of failure units and their lifetime are fixed irrespective of effective linewidth. This assumption results in a fundamentally different prediction from that of the physical model.

1.5.3 The effect of line length

The line length dependence of electromigration lifetime in wide Al lines was found by Agarwala et al. [73] to be a function of the linewidth. For wide lines, MTF decreases rapidly with increasing line length until the length is greater than 62.5 and 125 μm in Al lines of 10 and 15 μm width, respectively. Then, the lifetime reaches a saturation value beyond a critical length in the range of 125 μm to 250 μm and 500 μm , corre-

spondingly. DTF also decreases with increasing line length. For narrow Al-Cu lines of 0.75 μm width, MTF and DTF decrease slightly as line length increases from 10 to 50 μm and then level off at a line length of 500 μm [76].

The statistical model presented in the previous section may explain the linewidth dependence of MTF and DTF. The probability of finding weaker failure units is higher and more uniform in a longer line, i.e., N_s of either eq. (37) or eq. (38) increases, and, hence, MTF and DTF decreases.

1.5.6 The effect of alloying elements

It is well known that the addition of Cu up to 4 % increases MTF by more than an order of magnitude compared to pure Al [24]. As summarized in Table 1.2, the same effect was found with the addition of Mg, Ni, Cr and Ti, while Si, Au and Ag have no apparent effect on the electromigration lifetime. Among these alloy systems, the Al-Si and Al-Cu-Si systems are commonly used for the applications. The reason for the addition of Si is to prevent junction spiking due to interdiffusion of Si from the substrate to Al interconnects [86]. Although there are better alloy systems than Al-Cu-Si, the usefulness of other alloys is restricted by their complexity and other undesired properties [83].

The beneficial effect of substitutional solutes on MTF is superficially surprising, since it has been shown that Cu and Mg, and most other substitutional alloy elements actually increase net diffusion in the presence of a high current density (see section 1.2). Since voids grow by the coalescence of vacancies, the increase in the rate of substitutional diffusion should, superficially, enhance void growth and promote failure. In order to explain this discrepancy, several mechanisms were suggested [71, 87-95]. Since it was found that grain boundary electromigration of Al atoms is actually reduced by the presence of solute atoms, these mechanisms concern the interaction between grain boundary electromigration and solutes.

Table 1.2 Effect of alloying elements on the MTF of electromigration failure.
MTF was normalized by MTF of pure Al (30-45 hrs).

Alloy (wt %)	MTF	Comments	Reference
Al	1		[77]
Al-1.8 Si	1	no influence	[77]
Al- 2 Ag	1	no influence	[78]
Al -2 Au	1	no influence	[78]
Al-4 Cu	75	MTF is maximum at 6 % of Cu.	[24, 78]
Al-4Cu-1.7 Si	90		[79]
Al-3 Mg	33	Mg conc. less than solubility limit has little effect on MTF	[80, 81]
Al-2 Cr	270		[80]
Al-2 Ni	40		[82]
Al-4Cu-2Ni-1.5Mg	1000	quaternary alloy	[83]
Al- 2 Cu- 0.3 Cr	2000	bamboo grain	[84]
Al- 0.15 Ti	100	MTF depends on linewidth.	[85]
Al-0.1 Cu-0.15 Ti	150	Ti increases the resistivity.	

First, it was suggested that the solutes segregate to grain boundaries and preferentially bind with vacancies, thus increasing the activation energy of grain boundary electromigration, which accounts for the improvement of electromigration resistance [87-92]. Second, the beneficial solutes are added in concentrations that exceed the solubility limit. The resulting precipitates may act as vacancy sinks, diffusion barriers, or preferential sites for void nucleation [93-95]. Third, Nix and Artz suggested that solutes increase the mechanical strength of the film [71]. Electromigration introduces internal stress as discussed before. Higher mechanical strength may impart a greater resistance to grain

boundary electromigration and void formation. None of suggested mechanisms can provide a feasible explanation for all experimental observations, regarding the effect of solutes on grain boundary electromigration. A complete theory must explain the following:

1) The electromigration rate of Al decreases in the presence of certain solutes such as Cu and Mg, which contradicts the result of lattice electromigration. The quantitative determination of the effect of Cu on the flux of Al electromigration, obtained by electron probe analysis, showed that the Cu addition reduces Al grain boundary electromigration by a factor of about 80 [39]. Also, the cross strip experiment [20, 96], as shown in Fig. 1.10, qualitatively confirmed the estimation; the flux difference between Al and Al-Cu causes voids and hillock formation, and their polarities indicate a reduction of Al electromigration in the presence of Cu. It was also observed that voids form in the Al-Cu alloy when the concentration of Cu is reduced to the solubility limit.

Fig. 1.10 A schematic illustration of cross strip technique used to compare the electromigration flux of Al atoms in pure Al and Al-Cu alloys.

- 2) Solute migrate preferentially, while they retard the migration of Al atoms. Various studies reported that Cu preferentially migrate in the direction of electron flow [21-23].
- 3) It is often observed that voids form after the depletion of solute atoms. *In situ* SEM observation of electromigration in Al-Cu-Si interconnects revealed that voids formed after complete depletion of Al-Cu precipitates [21].
- 4) Some alloy elements such as Ag and Au have little influence on the electromigration lifetime, although they preferentially bind with vacancies and form precipitates like other

elements [24].

1.6 Objective and approach of this thesis

This thesis has two main objectives. As discussed, studies on the electromigration failure in interconnects of Al and Al alloys are extensive; however, these studies are mainly confined to the failure mechanism of wide interconnects, $\sim 10\text{ }\mu\text{m}$ width [97]. The failure mechanism in narrow lines has not been well characterized. Also, the effect of solutes on the electromigration failure mechanism is still not clear. These two main questions are explored in this thesis.

The most direct way to study the failure mechanism is through high-resolution microscopy of lines that have been treated to control microstructure and tested to failure in a way that preserves the failure site. For this purpose, a typical alloy system (Al-Cu-Si) was chosen, and the interconnects with various linewidth were prepared. In order to investigate the effect of solutes on the electromigration failure, low temperature aging was used because it allows control of the state of solutes through precipitation, without disturbing the grain structure. Then, these lines were tested to failure, and the failure morphology and lifetime statistics were investigated. Through these observations, it was possible to establish the failure mechanism of interconnects and its interaction with solutes.

The experimental technique is described in chapter 2. Chapter 3 describes the microstructure change of Al-Cu-Si thin films with aging treatments, characterized through TEM observation and electrical resistivity variations. The variation of the electromigration lifetime and the failure mechanism with the variation of microstructural factors including pre-aging condition is explored in chapter 4. Since it was found that the Al-Cu precipitate interacts with the electromigration, the mechanism of electromigration in the presence of Al-Cu precipitate is discussed in chapter 5. In chapter 6, a statistical model

of electromigration failure is introduced, based on the experimental findings in this study. The general aspects of statistics and the brief discussion of stress effects in thin films are introduced in the Appendices A and B.

CHAPTER 2

EXPERIMENTAL TECHNIQUE

2.1 Thin Film Deposition and Sample Preparation

The alloy used for this research was Al-2Cu-1Si (composition in weight percent), which is commonly used for Al lines in microelectronics devices. The Si is added to retard diffusion from the Si substrate; prior research suggests that this level of Si has a negligible effect on electromigration lifetime [79].

The main experimental samples were made by depositing 0.5 μm films onto a 100 mm silicon substrate with a (100) surface that was coated with 0.05 μm of thermally grown oxide. In order to obtain various grain structures, films were deposited under two different conditions: 450°C under a 100 V bias voltage ("planarizing condition") and 30°C under a no bias voltage. Prior to line patterning, some of the samples were furnace annealed (FA) at 425 °C for 30 minutes in a forming gas environment, and others were given a rapid thermal anneal (RTA) that involved heating to 500°C for 1 minute, followed by quenching. These treatments were intended to homogenize the solute.

In order to prepare the lines for electromigration tests, standard lithographic and plasma etching techniques were used, and two different types of test line structures were patterned as shown in Fig. 2.2: an array structure with 25 parallel lines and a "single line" structure with eight individual lines per test chip. All lines were 800 μm in length. The parallel array test structure was used in order to obtain lifetime data and statistics in a single test. The single line structure was used for detailed studies of failure mechanisms. Some of the single line structures were patterned to contain only one test line per test chip

and were 1000 μm in length, and these lines were used to study the electrical resistivity variation due to precipitation. The parallel test line structure contained inert lines (no electrical current) which were used to separate the effects of electromigration from the effects of thermal exposure during the test. Test lines were patterned with nominal widths of 1.3, 2, 4 and 6 μm .

Fig. 2.1 Schematic representations of the thin-film test structures: (a) array structure with 25 lines, (b) single line structures.

2.2 Electromigration Test

In order to test the electromigration lifetime of a sample, the test chip was placed on a hot chuck and was subjected to a current input. During the test, the voltage across the sample lines was monitored and recorded. Figure 2.2 shows a schematic diagram of the test circuit for the array line structure; the circuit consists of a probe station with a hot chuck, a DC power supply, a multi-channel voltage scanner and a computer. Provided that the resistance of the i^{th} test line is r_i , the total resistance of 25 lines in parallel connection, R , is given as

$$R = \left(\sum_{i=1}^{25} \frac{1}{r_i} \right)^{-1} \quad (2.1)$$

Then, from Ohm's law, the total amount of current applied, I_t , becomes

$$I_t = \frac{V}{R} = V \sum_{i=1}^{25} \frac{1}{r_i}. \quad (2.2)$$

Since the resistance of each line, r_i , is presumably the same for all 25 lines, each line is under the same current, $I_i = I_t / 25$, and the failure of any line decreases the total current by I_i . Hence, the time to failure of the lines can be determined by monitoring the change of the total current. However, as will be discussed in later sections, the electrical resistance of samples used in this investigation were not a constant but decreased about 10% with time due to resistivity decay by precipitate reconfiguration; the applied current increased, accordingly. To eliminate this effect, the current was monitored, and the voltage was adjusted every 50 seconds to maintain a constant current.

A single line structure was tested in a manner similar to the array line structures. In this case, a power supply with eight independent constant current sources was used, and voltage across each line was monitored. Using Ohm's law, the resistance change was calculated and was used to determine the time to failure.

Fig. 2.2 Electromigration test circuit; this circuit is for the 25 line array structure. For the single line structure, a DC supply with multi-channels was used.

2.3 Electrical Resistivity Test

The samples used in this study initially contained a considerable amount of super-saturated Cu. Upon testing, which was mostly done at 225°C, a rapid precipitation of Cu happened, and the electrical resistivity decreased correspondingly. Since it was found that the kinetics and the amount of the electrical resistivity can provide useful information on the precipitation behavior in the samples, accurate characterization of the resistivity decay was attempted.

The line structure for this study was basically the same as the single line structure, except that the line length is 1000 μm . Samples were placed in a Perkin-Elmer furnace mechanism, which was originally designed for a differential scanning calorimeter, and a probe station, a constant current source, a voltage meter and a computer-regulated relay were arranged as shown in Fig. 2.3. The relay was used to minimize the effect from Joule heating and electromigration by allowing a current (0.1 mA) only during voltage measurements that were usually done every 300~500 seconds.

The temperature of the furnace was controlled within an accuracy of $\pm 0.1^\circ\text{C}$. It took less than a minute to reach the test temperatures, and, hence, precipitation during initial heating was minimized. Also, these samples were heated in an Ar atmosphere to prevent any possible oxidation.

Fig. 2.3 Schematic illustration of the circuit used for the electrical resistivity measurements.

2.3. Joule heating

The system introduced in section 2.2 was also useful to characterize the temperature rise due to Joule heating during electromigration test. Under the current density, j , the actual temperature of the lines, T , is higher than the ambient temperature, T_a , following the simplified relation as [98]

$$T \equiv T_a + \frac{\alpha \rho_0 j^2}{H} \quad (2.3)$$

where ρ_0 and α represent the resistivity of the film at T_a and the temperature coefficient of the resistivity, respectively: H is given by

$$H = \frac{K_u}{t_{Al} t_u} (1 + 0.88 \frac{t_u}{W}) \quad (2.4)$$

in which K_u is the thermal conductivity of the underlayer, t_{Al} is the film thickness, t_u is underlayer thickness, and W is the test linewidth.

Fig. 2.4 An example of the increase in the electrical resistance with current density due to Joule heating in the 2 μm wide lines.

Eq. (2.3) is useful when the electrical resistivity of film is known and constant; however, the resistivity of films in this study was varied from sample to sample and also decreased with time. Hence, the temperature increase of the samples were indirectly characterized using the electrical resistivity variation with current density. For this purpose, the system introduced in section 2.3 was used. Initially, samples were aged until the resistivity decay from the precipitation practically stopped, and then the resistance of the line was monitored at various substrate temperatures as a function of current density. A typical example of this test performed on a 2 μm line is shown in Fig. 2.4.

Based on the test results, the current densities for the electromigration test were chosen to have a temperature rise less than 10°C, and the temperature difference was compensated by adjusting the substrate temperature.

2.3 Characterization

The principal characterization tools used in these tests were scanning electron microscopy (SEM), which reveals the superficial morphological features of line damage and failure, and transmission electron microscopy (TEM), which reveals microstructural details such as the grain size, the precipitate size and distribution, and the microstructural features of the damage and failure sites. To create specimens for TEM analysis, 3 mm discs were mechanically thinned to a 100 μm thickness from the Si substrate side and were then dimpled and ion milled to produce an area thin enough for transmission. Unpatterned samples were examined to determine the initial grain size; the reported values are averages of measurements of more than 200 grains. Failed samples were studied to determine the failure mode. TEM specimens of failed lines were prepared by the same technique as unpatterned samples. However, in order to preserve failure morphology, the underlying oxide, which can mechanically support the failed lines in thinned areas, was not removed. The sample preparation technique to achieve the required sample condition is schematically illustrated in Fig. 2.5. In this technique the thickness of each step was

controlled by the optical properties of Si: Si becomes transparent when its thickness is less than $10\text{ }\mu\text{m}$, and its color changes from dark red to bright yellow with decreasing thickness.

(a) After Dimpling

lines are visible with the background color of dark red under light

(b) High angle ion milling ($18\sim 20^\circ$ for 30 minutes)

lines are visible with the background color of bright yellow under light

(c) Low angle ion millig (10° for 2 hours)

lines are visible with no background color

Fig. 2.5 The technique for TEM sample preparation of failed lines.

CHAPTER 3

PRECIPITATION IN THIN FILMS

Most Cu alloyed in Al interconnects exists as a form of Al-Cu precipitate, since the solubility of Cu in Al is extremely low. In order to understand the mechanism by which the addition of Cu retards the electromigration-induced damage, therefore, precipitates and their interaction with electromigration should be considered. This chapter addresses the characteristics of precipitation in Al thin films to provide basis for further investigation on the relation of alloy elements and electromigration failure. Precipitation in Al-Cu alloys is well studied [99-101]; however, precipitation in thin films has not yet been characterized yet. Unlike bulk alloys, thin films have large surface areas and relatively small grains; these microstructural characteristics of thin films should influence the precipitation.

The precipitation behavior of the thin films was characterized in two ways. First, samples were aged for various times at 225°C, and precipitate evolution was characterized under TEM. Second, the electrical resistivity was monitored during aging at various temperatures, including 225°C, which allowed for the characterization of precipitation kinetics. The electrical resistivity was useful in investigating the precipitation characteristics in thin films because the grain boundary density and the fraction surface of area could be easily changed by adjusting line width for a given microstructure. These two observations were analyzed and incorporated into the quantitative description of precipitation behavior in thin films. The predominant role of grain boundaries on precipitation in thin films is reported in this chapter. Overall observations are presented in the first three sections, and they are discussed in the last three sections.

3.1. As-received microstructure

3.1.1 Grain structure

The usual deposition mechanism, growth and coalescence of nuclei followed by nucleation, played a role in determining the grain structure of the samples [102]. Since the nucleation and growth of grains are thermally activated processes, the grain structure in the as-deposited samples was influenced by the substrate temperature during deposition. Fig. 3.1 shows a comparison of grain structures of as-deposited samples. The sample deposited at 30 °C contained fine and randomly oriented grains, while the sample deposited under the planarizing condition contained relatively large and preferentially oriented, $\langle 111 \rangle$, grains.

Subsequent heating of these samples changed the grain size in two ways, depending on the initial grain structures: grain growth and grain refinement. Heat treatment of samples deposited at room temperature induced extensive grain growth, while slight grain refinement was found in the samples deposited under the planarizing condition. Grain size distribution for samples that was deposited under the planarizing condition, and samples deposited at both conditions and RTA heat treated is compared in Fig. 3.2, in which grain size is plotted as a function of cumulative probability. It can be seen that the grain size generally follows a log-normal distribution, which is common in thin film structure [103]. The standard parameters of the grain size distribution are the mean (G_{50}) and shape parameters (σ) of the log-normal distribution, and are summarized in Table 3.1. Note that the mean grain sizes increase during the heat treatment of samples deposited at room temperature, while the opposite is true in samples that were deposited under the planarizing condition.

The grain growth that is found in heat treated samples deposited at room temperature is the expected result. The rate of grain growth is time dependent, and, hence, when heating time is short, as in RTA treatment, an abnormal grain growth can be promoted.

Fig. 3.1 TEM micrographs showing the typical microstructure of films deposited (A) under the planarizing condition and (B) at room temperature. (top: XBB 933-1218, bottom: XBB 933-1217)

Fig. 3.2 The cumulative distribution of the effective grain size for films processed in various ways.

Fig. 3.3 Al-Cu phase diagram showing the metastable GP zones, θ' and θ'' solui.

This abnormal grain growth can be seen from the grain size distribution of the sample deposited at room temperature and subsequently RTA heat-treated, which is presented in Fig. 3.2, where the grain size distribution deviates from log-normal distribution at the right tail [104]. Since the short period of heating (1 min.) was not long enough to promote a steady state grain growth, it produced abnormal grain growth, resulting in a few large grains surrounded by many small grains. On the other hand, the grains in the sample deposited under the planarizing condition were initially stable and large. Thus, subsequent heating did not produce much grain growth. Instead, it appears that polygonalization or recrystallization induced by the thermal stress promoted the grain refinement; this is discussed further in detail in Appendix B.

Table 3.1 The estimated parameters of the grain size distribution, characterized as the mean (G_{50}) and shape parameter (σ) of the log-normal distribution.

Deposition condition	Heat Treatment	G_{50} (μm)	σ
450°C, 100 V	None	2.4	0.50
	RTA	2.04	0.41
	FA	2.18	0.38
30°C, 0 V	None	<0.4	-
	RTA	0.91	0.48
	FA	1.52	0.41

3.1.2 Initial precipitation

Since film processing was done at a temperature where the Cu in the film is soluble, as can be seen from the phase diagram of Al-Cu alloys in Fig. 3.3 [105], any Cu-containing precipitates that are present in the initial microstructure formed during cooling. Very few precipitates were found in either the as-deposited (Fig. 3.1) or the RTA films. A low density of small precipitates, however, is present in the initial state of the FA films. These are predominantly θ -phase precipitates that appear to have nucleated at

Fig. 3.4 TEM micrographs showing typical microstructures of the films deposited under the planarizing condition after (A) RTA and (B) FA treatment. (top: XBB 933-1221, bottom: 919-7581)

grain boundaries, free surfaces, and heterogeneous sites within the grain during the relatively slow furnace-cool from the aging temperature. The typical TEM microstructure of RTA and FA samples is shown in Fig. 3.4.

All samples investigated in this study contained a few Si precipitates, primarily located at grain boundaries. Since the processing temperatures, 500°C and 450°C, were not high enough to dissolve the Si completely [106], a small number of Si precipitates existed even after cooling. It is well known, however, that the solubility of Si in Al is significantly enhanced by the presence of Cu [107], and, therefore, the precipitation of Si during subsequent heating at lower temperatures would not be significant. In fact, no significant precipitation of Si was observed during the course of this investigation. Therefore, the precipitation behavior of these samples during aging was observed to be essentially the same as that in Al-Cu alloys.

3.2 Precipitation during aging

The normal precipitation sequence in an Al alloy that is supersaturated with Cu is a three-step sequence in which the Cu first clusters into "GP zones" of roughly nanometer size. These are superseded by metastable, θ' precipitates that have an equilibrium Al_2Cu composition, but with a tetragonal crystal structure that is coherent with the matrix along the broad faces of the thin plates in which it forms. These are ultimately replaced by larger, incoherent precipitates of the equilibrium phase, $\theta(\text{Al}_2\text{Cu})$ [99-101]. The precipitation of the θ phase is strongly catalyzed by grain boundaries, which is where these precipitates tend to appear [22, 93, 94, 102, 103]. In the present study no attempt was made to locate GP zones. Emphasis was on the precipitation and coarsening of the θ' and θ phases.

While there was a low density of small θ -phase precipitates in the initial state of the FA sample, and unresolved GP-zones were almost certainly present in all samples, the

significant precipitation and coarsening occurred during low-temperature aging at 226°C. TEM studies showed that the precipitation and coarsening behavior is essentially the same for all films. The first observable precipitates are θ' , which densely decorate the interiors of the grains as illustrated in Fig. 3.5. These θ' phase precipitates were observed even in samples aged for 5 minutes. θ -phase precipitates form on the grain boundaries, and create precipitate-free zones along the boundaries. As aging proceeds the precipitate distribution changes in three ways, which are illustrated in Figs. 3.6 and 3.7. The θ precipitates in the grain boundaries coarsen rapidly, particularly at three-grain junction lines (Fig. 3.6), the θ' precipitates in the grain interiors gradually disappear, and θ precipitates replace θ' in grain interiors (Fig. 3.7). The important observation is that the coarsening of θ' was not taking place homogeneously but was affected by the grain size. For example, different microstructures of the sample that was deposited at room temperature and RTA heat treated are compared in Fig. 3.8, where TEM microstructure of the film before aging is compared with that of the film aged for 4 hours. Notice that the large grains are decorated with fine θ' precipitates while a smaller number of θ' precipitates are visible in the small grains. On further aging the θ precipitates in the grain interiors are gradually consumed by those in the grain boundaries, and the latter also coarsen at the expense of one another. After 48 hours aging there is a small residual density of θ precipitates within the grains and a distribution of relatively large precipitates at grain boundaries.

The measured densities of θ and θ' precipitates taken from more than 50 grains of samples that were deposited under the planarizing condition and subsequently heat treated are plotted in Fig. 3.9. Note the virtual disappearance of θ' after 24 hours aging, and the maximum in the density of θ precipitates at that time. The density of intragranular precipitates in the 24 hour specimens increases with the grain size. Analysis shows that there are approximately 24 ppts./grain in samples aged from the as-deposited condition, 18 in those aged from the FA condition, and 17 in those aged after RTA.

Fig. 3.5 TEM micrographs showing the image of θ' precipitates formed in a RTA sample that was deposited under the planarizing condition and aged for 2 hours: (A) planar view, and (B) cross-sectional view under bright field and dark field conditions. (XBB 933-1219)

Fig. 3.6 TEM images of grain boundary θ after (A) 2 hours and (B) 7 hours of aging in the film that was deposited under the planarizing condition and RTA treated. (XBB 926-4151) .

Fig. 3.7 Bright filed and dark filed TEM images θ' precipitates taken after (A, C) 2 hours and (B, D) 7 hours of aging. These are the same films that are shown in Fig. 3.6. (XBB 933-1220)

Fig. 3.8 TEM micrographs comparing the microstructure of a film deposited at room temperature and RTA treated (A) before aging and (B) after 4 hours of aging at 225°C. (XBB 932-699)

Fig. 3.9 The type and density of intergranular precipitates as a function of aging time.

Fig. 3.10 A plot showing the resistivity decay at 225°C for 6 μm wide lines.

Two other features of the coarsening process are significant. First, while both Cu and Al migrate by exchanging with lattice vacancies, the net effect of substitutional diffusion during normal aging is the exchange of Cu and Al. When Cu-rich precipitates dissolve they are replaced by Al matrix; no Kirkendall voids are formed. Second, at this low temperature there is little or no grain coarsening. The mean grain size is unaffected by the aging process.

3.3 The electrical resistivity decay during aging

The electrical resistivity of samples with various linewidths was monitored using the technique introduced in section 2.3. Samples were placed in a furnace and heated at 195, 200, 215, 220, 225 and 230°C. Then the change of electrical resistivity was measured until the variation became practically zero. Since it was found that samples deposited under the planarizing condition and RTA treated samples deposited at both conditions were most appropriate for precipitation study, test results on those samples are presented here. For simplicity, each sample is noted as a symbol from now on; A: samples deposited under the planarizing condition, B: RTA of sample A, and C: RTA of sample deposited at room temperature.

The electrical resistivity of the samples contained a general decay trend: as soon as the test was started, the resistivity of samples A, B and C, started to decrease exponentially from the initial value $\rho(0)$ to an asymptotic value $\rho(\infty)$. A typical example of the resistivity decay found at 225°C on 6 μm lines is shown in Fig. 3.10. In this figure, the resistivity is referenced to the initial value as $\rho(t)/\rho(0)$, namely relative resistivity. It was found that the decay curves shown in Fig. 3.10 can be divided into two elemental factors: the kinetic factor and the scale factor. The kinetics factor represents the decay rate to the saturated resistivity. By normalizing the resistivity to scale it from 0 to 1 as

$$\varphi(t) = \frac{\rho(t) - \rho(\infty)}{\rho(0) - \rho(\infty)} \quad (3.1)$$

where $\rho(t)$ represents the resistivity of the sample at time t , the decay kinetic of samples can be directly compared. The scale factor is the factor that determines the amount of decay during the test. This factor is not influenced by the decay kinetics, and it is determined from the asymptotic value of the resistivity, $\rho(\infty)/\rho(0)$. For example, the total decay of samples B and C is more than that of sample A. The scale factor can be easily obtained by measuring the total amount of the decay during the test, defined as

$$\beta = \frac{\rho(0) - \rho(\infty)}{\rho(0)} \quad (3.2)$$

Introducing the above two factors, the decay curves were analyzed. The normalized decay curves of the data shown in Fig. 3.10 are shown in Fig. 3.11. Figure 3.11.B shows the semi-log scale plot of $\varphi(t)$ for clarity. It appears that the decay is the slowest in sample A and the fastest in sample C. The decay curve of sample C shows an interesting feature. The decay is initially the fastest, but after 90% drop in the value of $\varphi(t)$ the decay rate slows considerably.

The kinetic difference and characteristic shape of the curve are not affected by the test temperature; simply it takes a longer time to reach the same value of $\varphi(t)$ as the test temperature decreases. Hence, it is possible to estimate the activation energy of the decay kinetics by defining a scale factor χ which normalizes the time axis. The time axis of $\varphi(t)$ tested at 230°C was set as the reference, and the time axes of $\varphi(t)$ tested at other temperatures were reduced by a factor of χ until they matched. The estimated χ showed Arrhenius type behavior, and the estimated activation energy was 1.38 ~1.42 eV.

The kinetics factors were also analyzed for samples with narrower linewidth, 1.3 μm . It was found that the decay kinetics in samples with 1.3 μm width is slower than that in samples with 6 μm width. The effect of the linewidth was most pronounced in sample

Fig. 3.11 The normalized decay curve, $\varphi(t)$, taken from data shown Fig. 3.10: (a) linear scale, and (b) semi-log scale.

Fig. 3.12 The effect of linewidth on the resistivity decay at 225°C for lines deposited under the planarizing condition: (a) decay curve, and (b) semi-log plot of kinetics factor, $\phi(t)$.

A, and the typical test result found at 225°C is shown in Fig. 3.12, showing the decay curves (A) and the corresponding $\varphi(t)$ with semi-log scale. It can be seen that the decay is slower in the 1.3 μm sample, while both showed the same total decay amount. This decay retardation in narrower lines was observed in every test temperature and sample. It was also found that the time-scale factor χ in samples with 1.3 μm width showed the similar activation energy as samples with 6 μm width.

As defined in eq. (3.2), β is a measure of the total amount of resistivity decay during the test. It was found that β is affected by the initial condition of the samples and the test temperatures. The effect of the initial sample condition on β was already shown in Fig. 3.10: the amount of decay in sample A is considerably smaller than those of sample B and C, while sample B and C show a similar amount. As the test temperature decreased, β increased. Also, it was found that the effect of test temperature is closely related the solubility limit of Cu. The estimated β for each sample is shown in Fig. 3.13 as a function of solubility limit of Cu at the test temperatures. There exists a good correlation between β and the solubility. Also, β of sample A is always lower than those of the others, and β of samples B and C are almost identical at every temperature.

3.4 Precipitation in Thin Films

As shown in TEM investigations of aged microstructures, the precipitation behavior in thin films is essentially the same as that in bulk alloys. As in bulk alloys, coherent GP zones form and rapidly coarsen to θ' phase in less than a few minutes at 225°C. These θ' precipitates ordinarily would coarsen and ultimately become replaced by θ precipitates; however, it was found that these θ' precipitates were rapidly consumed to the grain boundary. Consequently, grains become relatively precipitate free with aging. This process is more rapid in smaller grains. Even the surviving θ precipitates within grains virtually disappear when the samples are overaged.

Fig. 3.13 The measured scale factor, β , as a function of Cu solubility.

These results can be attributed to the existence of a diffusion field toward the grain boundary. A grain boundary provides an easier nucleation site for precipitation due to its lower energy barrier. Therefore, θ phase forms at grain boundaries immediately after aging starts. The concentration of Cu at grain boundaries is close to the equilibrium concentration due to the presence of equilibrium θ phase. On the other hand, the interiors of grains, where meta-stable θ' -phase precipitates form, initially contain a considerable amount of supersaturated Cu. The chemical potential difference between the meta-stable and equilibrium phases causes θ' precipitates to dissolve: Cu migrates to precipitate in grain boundaries. If the grain size is large enough that most θ' precipitates are far from the grain boundary, then the normal coarsening process can take place; the θ' particles grow by consuming each other. On the contrary, if the grain size is small, as it is in thin films, normal coarsening is overcome by the diffusion field imposed by the grain bound-

ary, and, therefore, intragranular precipitates dissolve while grain boundary precipitates grow. This grain boundary effect on precipitate evolution provides a qualitative reason for the rapid disappearance of θ' precipitates and the grain size dependence of its kinetics in thin films.

The effect of grain boundaries on the kinetics of precipitate evolution can be quantitatively modeled using a conventional diffusion model that has been frequently used in many other similar studies [93, 108, 109]. This model assumes that there is no concentration gradient along the thickness direction, and that concentration of Cu in grains is initially uniform, C_i . Then, assuming a cylindrical grain with radius r_o , the diffusion of Cu in a grain can be given as

$$\frac{dC}{dt} = \frac{d}{dr} \left(\frac{1}{r} D \frac{dC}{dr} \right) \quad (3.3)$$

with the boundary conditions

$$\begin{aligned} C(r, t) &= C_i \text{ at } t = 0, 0 < r < r_o \\ C(r, t) &= C_e \text{ at } t > 0, r = r_o \end{aligned} \quad (3.4)$$

where D and C_e represent the diffusivity of Cu in Al lattice and the equilibrium concentration of Cu, respectively. The solution of eq. (3.3) describes the out-diffusion of Cu to the grain boundary where the concentration is fixed, as schematically illustrated in Fig. 3.14.

The kinetic function of Cu out-diffusion in this situation can be obtained from the estimation of the average concentration of Cu in a grain, $\bar{C}$, and it is known to be

$$S(r_o, t) = \frac{\bar{C}(t) - C_e}{C_i - C_e} = \sum_{n=1}^{\infty} \frac{4}{\alpha_n^2} \exp\left(-\frac{\alpha_n^2 D t}{r_o^2}\right) \quad (3.5)$$

provided that the α_n s are the roots of $J_o(r\alpha_n) = 0$ where $J_o(x)$ is the Bessel function of the first kind of order zero [110]. Eq. (3.5) can be simplified further by taking the large time approximation, and it can be expressed as

Fig. 3.14 A schematic representation of the concentration profile in a grain during out-diffusion of Cu to the grain boundary.

$$S(r_o, t) \approx \frac{4}{\alpha_1^2} \exp\left(-\frac{\alpha_1^2 D t}{r_o^2}\right) \quad (3.6)$$

where $\alpha_1=2.405$. Now, the function $S(r_o, t)$ describes the out-diffusion kinetics which is measured by the ratio of the relative amount of available Cu in the matrix to the total amount of available Cu which can out-diffuse after infinite amount of time. As expected, the out-diffusion kinetics in a grain is an exponential function of grain size and time. In small grains, θ' precipitates would rapidly coarsen to grain boundary, while coarsening of θ' is slow in large grains. This kinetic difference of precipitates imposed by a grain boundary is directly related to the electrical resistivity decay, as will be discussed in the following section.

3.5 Resistivity decay

As proved in Appendix C, the electrical resistivity of dilute alloys is linearly proportional to the mean concentration of solutes in the sample:

$$\rho = \rho_{Al} + \kappa \bar{C} \quad (3.7)$$

where ρ_{Al} , κ and $\bar{C}$ denote the resistivity of pure Al, the correlation constant and the mean concentration of solutes in the matrix, respectively. Hence, when there is a solute

reconfiguration in alloys, the electrical resistivity decreases due to the reduced amount of solutes in the matrix; the electrical resistivity of Al-Cu alloys decays with precipitation except for an anomaly during GP zone stage, where an additional electron scattering from the fine size of precipitates is active, so called Mott scattering [111-113]. The test temperatures used in this investigation were relatively high, such that the effect from GP zones was insignificant due to their rapid transformation to θ' . Therefore, the electrical resistivity decay observed here came from the reconfiguration of precipitates in grains.

3.5.1 Scale factor, β

Combining boundary conditions for out-diffusion in eq. (3.4) and the corresponding resistivity, the scale factor of the resistivity decay can be readily expressed as

$$\beta = \frac{\rho(0) - \rho(\infty)}{\rho(\infty)} = k' \left(\frac{C_i - C_e}{C_e} \right) \quad (3.8)$$

where k' represents the proportional constant. Eq. (3.8) indicates that the scale factor β is influenced by both initial concentration C_i and equilibrium concentration C_e , and it explains the estimated β shown in Fig. 3.13. Since sample A contained a lower amount of initial supersaturated Cu due to slower cooling, β should be less than for samples B and C at a given test temperature. Also, at a given initial Cu concentration, β is greater at lower temperature because the solubility limit decreases as the temperature decreases. Although it is not presented here, the estimated β found in furnace cooled samples was significantly lower than that of samples studied here, which is the another example of the analysis given in eq. (3.8).

3.5.2 Kinetic factor, $\varphi(t)$

The kinetic factor $\varphi(t)$ in a single grain is the same as $S(r_0, t)$ in eqs. (3.5)-(3.6), combining the definition $\varphi(t)$ in eq. (3.1) and the corresponding resistivity in eq. (3.7);

however, thin films contain grains with various radii. In order to account for the grain radius distribution in $\varphi(t)$, it is necessary to estimate the total amount of Cu in a sample which contains many grains. Since each individual grain follows the kinetic relation in eq. (3.5), the total amount of available Cu remaining in a sample at time t , $M(t)$, is the summation of all Cu atoms in all grains:

$$M(t) = \sum_j \pi r_j^2 \lambda (C_j - C_e) S(r_j, t) \quad (3.9)$$

where λ represents the film thickness and r_j represents the radius of j^{th} grain. Here, it is assumed that the concentration is uniform along the thickness axis, so that the volume of the grain times the mean concentration provides the total amount of available Cu for diffusion. The total amount of Cu which can out-diffuse in an infinite amount of time, $M(\infty)$, is simply the same as eq. (3.9) without the $S(r_j, t)$ term because it is only determined by the initial concentration and final concentration. The ratio between $M(t)$ and $M(\infty)$ represents the relative out-diffusion kinetics in the sample and, therefore, it is equal to the normalized resistivity $\varphi(t)$:

$$\varphi(t) = \frac{M(t)}{M(\infty)} = \frac{\sum_j r_j^2 S(r_j, t)}{\sum_j r_j^2} \quad (3.10)$$

This expression can be transformed to a statistical form containing the grain size distribution function, $f(r_j)$, by dividing each numerator and denominator by the total number of grains. The result has a form

$$\varphi(t) = \frac{\sum_m r_m^2 f(r_m) S(r_m, t)}{\sum_m r_m^2 f(r_m)} \quad (3.11)$$

where r_m denotes the increment of probability density function of grain size, $f(r_m)$. It is clear that the decay kinetics in thin films is influenced not only by the mean grain size but also by grain size distribution, and the contribution of each grain on $\varphi(t)$ is determined by the area fraction of the grain to the total line dimension.

The physical consequence of eqs. (3.10)-(3.11) is well presented in the test results of sample C. As noted earlier, a sample C underwent abnormal grain growth which produced grain structure with a few large grains surrounded by many small grains; this grain structure is shown in Fig .3.2 and Fig. 3.7. It was estimated that the small grains occupied more than 90% of the line dimension, while the remaining 10% is a few large grains. This grain structure is directly related to $\varphi(t)$: the $\varphi(t)$ of sample C is initially fast up to 90% of the drop and slows down suddenly afterward. In small grains, the out-diffusion kinetics are fast, and, thus, the $\varphi(t)$ decays rapidly until the out-diffusion in these grains is practically stopped. After this, the decay must come from the large grains in which out-diffusion is much slower. Since the area fraction of these large grains is significant in spite of their small number, it is possible to detect the sudden transition due to the large grains. Comparing $\varphi(t)$ and TEM microstructures of the aged sample already shown in Fig. 3.7, the analysis introduced here is becoming more clear. The 4 hours of aging at 225°C corresponds to the 90% of the decay. It is clearly visible that the large grains are still well decorated with the fine θ' precipitates, while smaller grains are relatively free of any precipitate. If the number of relatively large grains is one or two such that the area fraction is small as it is in samples A and B, it would not be possible to detect the transition.

Note that the eq. (3.11) and eq. (3.12) become the same as eq. (3.5) when the thin film contains grains with an uniform radius. In this case, the large-time approximation of eqs. (3.11)-(3.12) becomes

$$\varphi(t) \approx \frac{4}{\alpha_1^2} \exp\left(-\frac{\alpha_1^2 D t}{r_o^2}\right) \quad (3.12)$$

Eq. (3.12) indicates that when the $\ln\varphi(t)$ is plotted as a function of time, it provides a straight line which contains information on the diffusivity. This is one of the most common methods that have been frequently used to determine the diffusivity of impurity atoms or vacancies in metal using electrical resistivity [114-118]. In this sense,

eqs. (3.10)-(3.11) do not differ from the conventional model of electrical resistivity decay and provide a more general solution which can be applied to the study on samples with many grains.

Provided that the free surface is as effective as a grain boundary for the nucleation of θ , there would not be as significant a difference in the decay kinetics difference as seen here. The thickness of film is uniform. Thus, the diffusion distance is fixed as film thickness, so that $\varphi(t)$ should follow a similar form to eq. (3.12), in which r_0 becomes the film thickness. Furthermore, a reduced linewidth for a given sample should produce faster decay kinetics. This assertion can be explained as follows: With a given grain structure, making a line with a width smaller than the mean grain size will usually result in a line containing mostly one single grain spanning across the width. Consequently, the grain boundary density decreases and the surface area-to-volume ratio increases. The test results show, however, that the decay kinetics were observed to be slower in 1.3 μm lines, which indicates that the reduction of grain boundary density has a predominant effect on the decay kinetics, and a free surface is not as effective as a grain boundary for precipitate nucleation. The retardation of decay kinetics is more pronounced in sample A because of the most significant reduction of grain boundary density in sample A due to its larger grain size.

3.6 Applications of the resistivity decay

The usefulness of the resistivity decay is well demonstrated in this study. The qualitative observation of precipitation characteristics in thin films obtained from TEM was supported by the measurement of the resistivity decay with quantitative techniques, and the relative importance of free surface and grain boundary on the nucleation was investigated using the decay kinetics. It was found that the study on the resistivity decay is also useful in two ways. First, the diffusivity of Cu in thin film Al lattice can be esti-

mated by measuring $\varphi(t)$ when the grain size distribution is available. Secondly, if the lattice diffusivity of Cu is known, the grain size of unknown Al thin films can be estimated. The first application was attempted using the data obtained in this study, and the second application is briefly introduced, as follows.

3.6.1 Determination of lattice diffusivity of Cu

At a fixed grain size distribution, the $\varphi(t)$ is simply determined by the diffusivity of Cu due to its contribution to $S(r_j, t)$ in eqs. (3.10)-(3.11). It takes simply longer time to decay the same amount as the temperature decreases due to slower diffusion in each grain; however, the shape of decay curve must be preserved provided that there is no grain size change. Since no grain growth was observed at test temperatures, the curves tested at different temperature should coincide by simply factoring the time axis by χ a scale factor, χ . This is what was observed. The time-factor, χ , show an Arrhenius equation because it physically represents the activation energy of Cu diffusivity. The estimated activation energy of χ in this study was 1.38~1.42 eV, indicating that it is in fact quite close to the activation energy of Cu diffusion in Al lattice, 1.32-1.41 eV[119-123].

Although the activation energy of Cu diffusivity in Al thin film is proven to be the same as that in the bulk, the diffusivity itself is still unknown. However, the diffusivity can be estimated using eqs. (3.10)-(3.11) and grain size data shown in Fig. 3.2. When eqs. (3.10)-(3.11) are integrated with respect to time, they have a physical meaning of the area, A , under the decay curve $\varphi(t)$ and it becomes only a function of D and the statistical parameters of the grain size distribution:

$$A = \int_0^\infty \varphi(t) dt = \frac{1}{D} \left(\sum_{n=1}^\infty \frac{4}{\alpha_n^4} \right) \left(\frac{\sum_i r_i^4}{\sum_i r_i^2} \right) \quad (3.13)$$

or

$$A = \frac{1}{D} \left(\sum_{n=1}^{\infty} \frac{4}{\alpha_n^4} \right) \left(\frac{\sum_m r_m^4 f(r_m)}{\sum_m r_m^2 f(r_m)} \right) \quad (3.14)$$

where

$$\sum_{n=1}^{\infty} \frac{4}{\alpha_n^4} = 0.125.$$

The area under the decay curve $\varphi(t)$ can be numerically calculated and then the diffusivity D is given as

$$D = \frac{0.125}{A} \left(\frac{\sum_i r_i^4}{\sum_i r_i^2} \right) \quad (3.15)$$

or

$$D = \frac{0.125}{A} \left(\frac{m'(4)}{m'(2)} \right) \quad (3.16)$$

where $m(4)'$ and $m(2)'$ are the fourth and the second moments of grain radius distribution, and they are defined in eq. (A.11). If the grain radius distribution is exactly log-normal, then from eq. (A.35), eq. (3.16) simplifies to

$$D = \frac{0.125}{A} r_{50}^2 \exp(6\sigma^2) \quad (3.17)$$

where r_{50} and σ are the median grain radius and shape parameter of log-normal distribution, respectively; D can be simply determined. The grains in this study slightly deviate from the log-normal distribution. Hence, the fourth and the second moments were numerically calculated using data shown in Fig. 3.2. Figure 3.15 shows the results of the diffusivity estimation, plotting the diffusivity as a function of temperature. In this figure, the diffusivity of Cu in bulk alloys extrapolated from the data in several references is included as dashed lines [119-122]. It appears that the Cu diffusivity in thin films is faster by more than an order of magnitude than that in the bulk alloys, while the activation energy is similar. The pre-exponential factor of the diffusivity, D_0 , estimated here is about

17~46 cm²/sec, while that in bulk alloys is 0.15~0.65 cm²/sec. Given the facts that the lattice diffusivity of impurity atoms in thin films is known to be faster due to higher density of defects than bulk and the existence of residual stresses, the higher pre-exponential factor of the diffusivity obtained here is not unusual. It should be noted that the increased lattice diffusivity in thin films found here is somewhat greater than that found in other studies in which lattice diffusivity in films is reported to be 3 to 10 times greater than in bulk [123]. The presence of Si in the lattice may have influence on the Cu diffusivity. Also, the assumption of cylindrical grains may have caused overestimation of the pre-exponential factor.

Fig. 3.15 The estimated bulk diffusivity of Cu in Al. The dotted lines represent the extrapolated diffusivities of Cu in bulk Al alloy.

Although the model developed here is somewhat simple, it provides simple way to estimated the lattice diffusivity of solutes in thin films with a reasonable accuracy,

which has not been much explored due to experimental difficulties.

3.6.2 Determination of the grain size distribution

As noted in eq. (3.11), the measured decay function $\varphi(t)$ contains information of the probability density function of grain radius, $f(r_m)$. If the increment of the grain radius is set to be r_k , then there exist linear equations at a test time t_k defined from eq. (3.11) as

$$\sum_{k=1}^N r_k^2 f(r_k) H_{kj} = 0 \quad (3.18)$$

where $H_{kj} = S(r_k, t_j) - \varphi(t_j)$, and N denotes the total number of increment r_k . The physical meaning of H_{kj} is the difference between the ideal decay value of a sample with homogenous grain size r_k at time t_j and the decay value of the actual sample with inhomogeneous grain sizes. Apparently, H_{kj} is zero when the test time, t_j , is zero because both $S(r_k, 0)$ and $\varphi(0)$ are 1. At a given non-zero test time, t_j , there exists only one r_k which makes H_{kj} zero. The magnitude of r_k which makes H_{kj} zero decreases as the test time t_j increases. Therefore, the linear equations defined by eq. (3.18) are linearly independent with no zero t_j 's. With the $N-1$ number of t_j and the requirement

$$\sum_{i=1}^N f_i = 1,$$

then eq. (3.18) can be rewritten as a $N \times N$ matrix form as

$$\begin{bmatrix} r_1^2 H_{11} & . & . & . & r_N^2 H_{N1} \\ r_1^2 H_{12} & . & . & . & r_N^2 H_{N2} \\ . & . & . & . & . \\ r_1^2 H_{N-1,1} & . & . & . & r_N^2 H_{N-1,1} \\ 1 & . & . & . & 1 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ . \\ f_{N-1} \\ f_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ . \\ 0 \\ 1 \end{bmatrix} \quad (3.19)$$

The probability density function f has a non-trivial unique solution, for N independent linear equations are given to N unknown variables. The matrix $[f]$ can be numerically calculated.

3.7 Summary

Precipitation in Al thin films containing Cu is fundamentally the same as precipitation in bulk alloys; GP zones initially form and grow to metastable θ' -phase precipitate, and ultimately transform to stable θ -phase precipitate. Relatively small grain size, however, places GP zones and θ' precipitates in a chemical potential gradient from the grain boundary where θ precipitate forms immediately upon aging. Since the rate of θ' precipitation is extremely rapid, grain boundaries have little influence on the initial precipitation. Later, the coarsening rate of θ' slows down and is overwhelmed by the chemical potential gradient to the grain boundary. Therefore, most of the θ' precipitates inside the grains dissolve and diffuse to the grain boundary, resulting in a continuous growth of θ at grain boundaries; grain boundaries play a major role on precipitation in thin films.

The coarsening of θ' precipitates to a grain boundary involves the diffusion of Cu to the adjacent grain boundary. Since the accumulation of Cu in the boundary of small grains is faster than in larger grains, and θ' precipitates disappear much more rapidly in small grains. This was demonstrated by both TEM observation of aged films and the variation of the electrical resistivity during aging. It was found that the kinetics of resistivity decay reflects the grain size and its distribution of film, as well as precipitation kinetics. Using a simple diffusion model, the precipitation characteristics in thin films was characterized, and the lattice diffusivity of Cu was estimated.

CHAPTER 4

MECHANISM OF ELECTROMIGRATION FAILURE

The mechanism of electromigration failure in Al thin film interconnects is strongly influenced by various microstructural parameters of such film. These parameters include alloying elements, grain size and distribution, preferred grain orientation, interconnect linelength and linewidth. Since all of these parameters interact with each other, it is necessary to test lines with controlled microstructures in which only one parameter is varied. For this purpose, pre-aging of test lines with various linewidths was performed to investigate the role of alloying elements on the failure mechanism and its interaction with the line structure. As discussed in the previous chapter, when samples are aged at relatively low temperature, precipitation occurs at grain boundaries and in the interiors of the grains. With aging time, only the types and distribution of precipitates changes. Electromigration testing as a function of aging time for a given line structure should, therefore, reveal the precipitate influence on the failure mechanism, leading to an understanding of the role of alloying elements.

Test results and the failure mechanisms are introduced in this chapter. The failure mechanism in wide lines was found to be the same as the conventional one [1, 2, 34, 91], i.e., voids nucleate and grow at grain boundaries and, eventually, coalesce with one another to break the line. The failure mechanism in narrow lines, however, was found to be fundamentally different from that in wide lines. Failure was often found to be transgranular, and appeared in the form of thin, slit-like voids or cracks that transversed the grain. High-resolution metallographic studies of the failure sites in narrow lines, in addition to failure time test results, suggested that failure occurs at metallurgical "weak links"

along the line. The "weakest link" that leads to failure is the longest polygranular segment in the line. This metallurgical result, taken in conjunction with a semi-quantitative diffusion model, yields a plausible explanation for the failure mechanism in narrow lines. In this chapter, the microstructural failure mechanism in narrow lines is focused on. The role of Cu and the statistical aspects of electromigration failure will be discussed in details in the following chapters. Test results and metallographic observations are presented in sections 4.1 and 4.2, and the failure mechanism and the diffusion models are explored in sections 4.3 and 4.4. Finally, in section 4.5, the role of Cu is briefly discussed.

Fig. 4.1 The microstructure of as-patterned lines with widths of (A) 1.3, (B) 2 and (C) 4 μm . These micrographs were taken from the sample deposited at planarizing condition after 7 hours of aging. (XBB 933-1215)

4.1 Test results of electromigration lifetime

The electromigration lifetimes of interconnect of the different linewidths were tested under various current densities, temperatures, and with the variation of pre-aging times. Samples deposited under the planarizing condition were the main samples used in this investigation because they provide various effective linewidths (W/G), 0.5~2.5, resulting from the largest mean grain size. Unless otherwise specified, the discussion refers to these samples. The microstructures of as-patterned lines are shown in Fig. 4.1, where examples of narrow lines ($W/G \sim 0.5$) and wide lines ($W/G \sim 2.5$) are compared. These lines are aged for 7 hours before the TEM sample preparation in order to reveal the grain boundaries. The narrow lines have a predominantly "bamboo" structure in which single grains span the line. Polygranular sections occasionally appear along the length. The wide lines have polygranular cross sections almost everywhere. These lines were tested at a nominal current density of 2.5×10^6 A/cm². Although some tests were also done at higher current densities, those results are not presented here because they are not sufficient to provide the value of a conventional current exponent. Those samples were used, however, for high resolution metallographic studies of failure sites.

4.1.1 Failure as a function of linewidth for unaged samples

Fig. 4.2 shows the cumulative probability of failure for the three linewidths tested in the unaged condition at a temperature of 225°C and a current density of 2.5×10^6 A/cm². In all three cases the cumulative distribution of failures is well fit by the log-normal distribution. The median time to failure (MTF) is indicated in the figure. The variance (DTF) of the distribution fixes the slope of the data in the figure. The MTF and DTF of these lines are summarized in Fig. 4.3, including the results from 4 μ m lines. Although it is not strong, there is a linewidth dependence of MTF and DTF of lifetimes, as found in other studies. Test results from other samples, that were deposited at the planarizing condition and subsequently FA and RTA treated, showed a similar trend.

Fig. 4.2 The cumulative distribution of failure times for lines of three widths, tested in the unaged condition at 225°C and 2.5×10^6 A/cm².

Fig. 4.3 The MTF and DTF variation with the effective linewidth for unaged lines.

4.1.2 Failure as a function of test temperature for unaged samples

Fig. 4.4 shows the median time to failure for 1.3 μm and 6 μm lines as a function of test temperature over the range 190°C to 235°C at a fixed current density of 2.5×10^6 A/cm². The MTF data are fit to an Arrhenius expression with an activation energy, E_a ,

$$MTF = \exp\left(-\frac{E_a}{kT}\right) \quad (4.1)$$

The result is $E_a \sim 0.93$ eV for the narrow lines, $E_a \sim 0.65$ eV for the wide lines. Of course, two data sets are insufficient to prove a change of activation energy with linewidth. However, the results obtained here are in agreement with prior research that shows similar behavior. Dreyer and Varker [72] determined the activation energy as a function of linewidth for Al-1.5Cu at $j \sim 2.0 \times 10^6$ A/cm², and found that the value decreased with linewidth from ~ 1 eV for W/G significantly less than 1 to ~ 0.6 eV for wide lines.

Fig. 4.4 MTF as a function of test temperature for unaged lines of 1.3 and 6 μm width, tested at $j = 2.5 \times 10^6$ A/cm².

4.1.3 Failure time as a function of pre-aging time

The kinetics of electromigration failure were tested as a function of pre-aging time at a substrate temperature of 225°C and a current density of 2.5×10^6 A/cm². The array lines were thermally aged at 225°C for various times before testing. The test results are illustrated in Figs. 4.5-4.7. Fig. 4.5 presents the failure statistics as log-normal plots of the cumulative fraction of failed lines as a function of the electromigration time. Fig. 4.6 illustrates the MTF variation with pre-aging time of these lines. Fig. 4.7 compares the MTF of single-line specimens as a function of the ratio of linewidth to grain size, W/G, for specimens tested both without aging and after aging for 24 hours. The data show that aging narrow lines prior to testing have a very strong influence on both the mean time to failure and the failure statistics. There is a measurable, but much smaller, effect on the behavior of the wide lines, as already shown in Fig. 4.3.

First consider the behavior of the wide-line arrays. Fig. 4.6 shows a small monotonic increase in MTF for pre-aging times up to 48 hrs. Fig. 4.5 shows that the increase in MTF is primarily due to an increase in the minimum time required to initiate failure; the time to first failure within an array increases monotonically with pre-aging time while the time required to fail all lines changes very slightly, if at all.

The behavior of the narrow-line arrays is strikingly different. The mean time to failure increases dramatically when the sample is pre-aged for 24 hrs, from a value below that of the wide-line array to a value that is more than an order of magnitude higher (Fig. 4.6). Fig. 4.5 shows the cumulative distribution of failure times for various pre-aging times. Pre-aging changes the distribution in two ways. First, the samples with longer failure times in each set can be fit to a log-normal distribution. This distribution governs at least the last 75% of the failures. At intermediate aging times, however, the first few failures require much longer times than is predicted by the log-normal fit to the long-term data. There is a distinct bimodal distribution at intermediate times as shown by

Fig. 4.5 A log-normal plot of the failure times with various pre-aging times for line widths of (A) 1.3 and (B) 4 μm .

Fig. 4.6 The MTF variation as a function of pre-aging time for 1.3 and 4 μm lines.

Fig. 4.7 Test results on single line samples showing the dependence of the MTF on linewidth in the unaged and optimally aged conditions.

the two lines in the figure. However, the beneficial effect of aging is sensitive to the aging time. If aging is continued to 48 hours the benefit is lost, and the MTF decreases to a value that lies below that of the unaged specimen.

The variation of MTF with the effective linewidth, W/G , is plotted in Fig. 4.7. The figure includes data from the as-deposited, RTA and FA single-line samples to provide a range of values of W/G , and compares behavior in the unaged and peak-aged (24 hours) conditions. Prior work by several investigators has documented a significant increase in MTF and DTF with W/G at small values of the latter [64-67]. The present results suggest that this increase is very sensitive to the microstructure, which is determined by prior aging. The aged specimens show a dramatic increase in MTF as W/G drops below about 0.5, while the unaged specimens show only a small increase over the same range.

4.1.4 Failure time as a function of pre-aging temperature

Tests similar to those above were done by pre-aging lines at different temperatures. Lines were pre-aged at 310°C and 190°C for various times, and tested at the same condition as in the previous studies: 225°C and a current density of 2.5×10^6 A/cm². The test results are shown in Figs. 4.8-4.9. Fig. 4.8 compares the MTF variation as a function of aging time for samples aged at 3 different temperatures. It can be seen that the MTF variation of lines aged at 310°C shows the same trend as lines aged at 225°C. The peak aging time in lines aged at 310°C is shorter (8 hours) than in lines aged at 225°C (24 hours), and the corresponding MTF is about 40% lower in lines aged at 310°C. On the other hand, the MTF of the lines aged at 190°C increases continuously and slowly within 48 hours of pre-aging time. Fig. 4.9 illustrates the lifetime distribution of the lines at peak aged conditions. Lines aged at 190°C are not included because peak aging was not reached in the time aged. The distinctive bi-modality of the lifetime distribution found in

Fig. 4.8 The MTF variation of 1.3 μm lines as a function of pre-aging time at three different temperatures.

Fig. 4.9 A cumulative distribution of failure times for 1.3 μm lines at peak aging conditions.

the lines aged at 225°C for 24 hours also appears in the lines that were aged at 310°C for 8 hours, although the bimodality is less apparent.

4.1.5 Resistance change during electromigration

When the electrical resistance of lines during electromigration is monitored, it is possible to investigate the failure kinetics of lines. When damage forms and grows by electromigration, the electrical resistance increases accordingly [124-126]. Using single line structures, the kinetics of failure were investigated, and the results can be summarized as follows.

First, as found in many similar studies, the electrical resistance increases rapidly before failure. Generally, rapid failure occurred when the resistance increase was as high as 15 %. Depending on linewidth and aging condition, however, the kinetics of the resistance change is very different. First, for unaged lines, failure occurs shortly after the electrical resistance starts to increase. Typical resistance changes during electromigration tests of unaged 1.3 and 4 μm lines are illustrated in Fig. 4.10. In both cases, the electrical resistance decreases initially because of precipitation, as discussed in the previous chapter. However, there is a noticeable difference between wide lines and narrow lines. For wide lines, the increase in resistance is rather continuous and slow, while for narrow lines the increase is relatively abrupt and rapid. In addition, the magnitude of resistance increase before failure is greater in the wide lines. As noted in the figure, the resistance in narrow lines shows an occasional healing process, i.e., the resistance decreases rapidly after a sudden increase. This healing process frequently appears in narrow lines, while that is rare in wide lines. The healing of damages during electromigration is interesting and has not been reported, although the healing of lines after complete failure was observed in several investigations [31, 127].

Fig. 4.10 A typical variation of the electrical resistance during electromigration test of unaged, (A) 1.3 and (B) 4 μm lines.

Fig. 4.11 A typical variation of the electrical resistance during electromigration test of pre-aged, (A) 1.3 and (B) 4 μm lines.

Aging induces distinctive change in failure kinetics, depending on the linewidth. As previously presented, for wide lines MTF linearly increases with aging time. It was found that this increase in lifetime is mainly a result of the slower kinetics of failure. Fig. 4.11 shows that the resistance change in 48 hours aged 4 μm lines increases at a slower rate than that in unaged lines. Compared to the change in unaged lines shown in Fig. 4.10, aged lines require longer time and a greater magnitude of resistance increase to fail the lines after damage starts. Also, notice that the characteristic healing process, which was visible in unaged narrow lines, appears in aged wide lines. For aged narrow lines, the failure kinetics are fundamentally different from wide lines and unaged narrow lines. The critical amount of resistance increase, where failure occurs rapidly, is roughly the same for every aging condition. The kinetics of the resistance increase required to reach critical resistance, however, is a function of aging time. The slow and gradual increase of the resistance in lines pre-aged for 24 hours can be seen in Fig. 4.11. For under- and over-aged lines, the resistance change is relatively the same as in unaged lines except during the initial decay; failures are followed by a sudden and rapid increase of the resistance.

4.2 Microstructural mechanism of electromigration

4.2.1 Precipitation and coarsening during electromigration

During electromigration tests the samples experience a current density of 2×10^6 A/cm² as well as a temperature of 225°C. The concurrent electromigration modifies the precipitation and coarsening behavior in three ways.

First, the rate of coarsening is significantly increased. While the relative coarsening kinetics have not been yet quantified, direct comparison between the lines that were exposed to current and the parallel reference lines that were current-free shows that intra-

granular precipitates dissolve much more quickly in the current. Grains are often swept free of precipitates after only a few hours of exposure.

Second, the pattern of coarsening is heterogeneous. Electromigration causes preferential transport of Cu in the direction of current flow. The grain boundaries are decorated by precipitates which act as sinks for the Cu. Within a given grain, precipitates that are downstream in the current disappear first, yielding a spatially inhomogeneous precipitate distribution.

Fig. 4.12 TEM micrographs showing void formation at a θ' precipitate site, tested in the unaged condition for 2 hours at 225°C and $2.5 \times 10^6 \text{ A/cm}^2$. The void is visible under bright field conditions (A) due to a normal absorption effect, while only θ' precipitates are visible under dark field conditions (B). (XBB 926-4150)

Third, the dissolving precipitates tend to be replaced by voids rather than by matrix material. The effect is most pronounced in the dissolution of intragranular θ' precipitates. Fig. 4.12 shows an example where a θ' precipitate is partially dissolved during

Fig. 4.13 TEM micrographs showing void formation at θ precipitates (A-b) in the grain boundaries and (A-a and B) in grains after 4 hours of testing at 225°C and 2.5×10^6 A/cm². (XBB 919-7583)

electromigration and the missing material has been replaced by a void. A similar phenomenon is observed during the dissolution of θ precipitates in grain boundaries in the later stages of coarsening. Fig. 4.13 shows an example of voids that appear on the grain boundaries of a thick line after exposure to current that are very similar in shape and distribution to the θ precipitates that are dissolved. An intra-granular void is also visible in this figure as noted. This effect is presumably due to the strong preference for Cu-vacancy exchanges during electromigration; as Cu migrates out of the precipitates, vacancies are left behind which coalesce into voids.

4.2.2 The microstructure of the failure sites

4.2.2.1 Wide lines

The microstructural mechanism of electromigration failure was investigated by examining failed lines with scanning and transmission electron microscopy. The mechanism of failure in wide-line samples (4 and 6 μm) is the same for all pre-aging times. Voids nucleate along grain boundaries, and gradually coalesce to form a continuous void that breaks the line. In this sense, the failure mechanism of wide lines tested in this investigation is conventional: grain boundary failure. However, there is one factor which differentiates the failure mechanism of wide lines in this study from that of pure Al. Figs. 4.14-4.15 compare the failure morphology of grain boundary failure in pure Al lines versus Al-Cu-Si lines. Pure Al lines were tested at a substrate temperature of 175°C under a current density of $5 \times 10^5 \text{ A/cm}^2$. When the failure morphology of pure Al lines were examined under TEM, it was seen that voids always initiated at the edge of the line and propagated inward following grain boundaries. On the other hand, voids in Al-Cu-Si alloys are not necessarily associated with the edge of the line, rather they are finely dispersed along the grain boundary. As presented in the previous section, voids tend to form at the sites where precipitates were located, and, therefore, many independent voids are

Fig. 4.14 TEM micrographs showing (A) grain boundary failure and (B) void formation (B) in pure Al lines, tested at 175°C and 2.5×10^6 A/cm². (XBB 932-598)

Fig. 4.15 TEM micrographs showing the nucleation voids at grain boundaries in Al-Cu-Si lines, tested in the unaged conditions at 225°C and 2.5×10^6 A/cm². (XBB 919-7582)

visible along the grain boundaries. These voids grow independently and coalesce to form a continuous void which causes the line to fail.

4.2.2.2 Narrow lines

Direct observation of the failure sites in narrow lines reveals a failure mechanism that is not only morphologically different from that found in wide lines, but changes qualitatively in samples that have been aged to maximize the MTF. With the single exception of 1.3 μm lines that were pre-aged for 24 hours, the narrow lines failed in a slit-like failure mode. Fig. 4.16 is an SEM micrograph that shows the typical morphology of this failure found in unaged 1.3 and 2 μm lines. The failure site consists of a void that extends part way across the line which is continued to failure by a thin, slit-like break. The failure sites contain a second feature: a void is always associated with a large θ -phase precipitate located a short distance from the void in the direction of the electron flow. In almost all of the samples studied the failure is this type; test temperature and current density did not change the failure morphology. Except for peak aged lines, the failure morphology is consistently the same. Fig. 4.17 shows the failure morphology of lines in under- and over-aged conditions. As can be in the SEM micrographs, the failure morphology is consistently the same. However, when the lines are peak aged, the failure morphology is qualitatively different, as is shown in the scanning electron micrographs presented in Fig. 4.18. In this case, there is no obvious void or slit at the failure site. The line simply thins locally until it eventually fails. The degree of thinning prior to failure appears to be sensitive to the original processing of the film from which the line is made. Fig. 4.18 compares failure sites in as-deposited and RTA material. The RTA material thins less prior to failure, and fails more quickly. In order to understand this failure mechanism, unaged lines were tested at various test temperatures and current densities, and lines pre-aged at 225°C were tested and extensively studied.

Fig. 4.16 Typical morphology of failure sites as seen in SEM; these micrographs are taken from 1.3 (top A and B) and 2 μm lines (bottom A and B) tested in the un-aged condition at 225°C and $2.5 \times 10^6 \text{ A/cm}^2$. Each void is associated with a θ -phase precipitate on the downstream side. (XBB 933-1214)

Fig. 4.17 SEM micrographs showing the failure mode evolution in 1.3 μm lines with aging time: (A) unaged, (B) 12 hours aged, and (C) 48 hours aged. (XBB 910-7577)

Fig. 4.18 SEM micrographs showing failure sites in the optimally aged as-deposited (A) and RTA (B) samples. Note that the failure is accompanied by local thinning of the line. (XBB 910-7576)

The second metallurgical feature of the failure morphology, i.e., the pairing of voids and a large θ -phase precipitates is not unique to the failure site. Failed lines typically contained many edge voids that had not propagated to failure at the time the line was broken. Almost all of these are also paired with downstream θ -precipitates. The difference is that the separation between the pair is less than it is at the failure site.

To identify the metallurgical characteristics of these void-precipitate pairs and the location of void, high-resolution TEM studies were performed. Fourteen failure sites and 17 partially grown voids (we shall call these "damage sites") were successfully identified. The microstructure of the failure morphology in narrow lines is illustrated by the TEM micrographs shown in Fig. 4.19 and the schematic drawing in Fig. 4.20. The first important observation is that the voids are not normally located at the grain boundary, but are almost always transgranular. Second, in every case studied the void and precipitate bracket a polygranular segment of the line; the void appears in the bamboo grain that is the upstream boundary of the polygranular segment while the precipitate appears in the boundary of the bamboo grain that terminates the segment on the downstream side. The damage sites also share a second metallographic feature. While small, θ -phase precipitates are densely distributed along the line, there are none in the space between the paired void and θ -precipitate.

These observations suggest that electromigration failure in narrow lines occurs in the bamboo grain at the upstream end of a polygranular segment, that failure happens after Cu has been swept from both the polygranular segment and at least the downstream portion of the bamboo grain, and that the time to failure decreases as the polygranular segment becomes longer. The "weak links" in the line are polygranular segments, and they become weaker as they become longer.

Fig. 4.19 TEM images showing the typical microstructures associated with (A and B) damaged and (C) failed sites. The transgranular slit void and precipitate bound a polygranular segment. The region between the void and the precipitate is precipitate free. (XBB 926-4148)

Fig. 4.20 Schematic representation of the microstructure at a typical damage site. An edge void and precipitate bound a polygranular segment. Both the polygranular segment and the bamboo grain that contains the void are precipitate free.

4.2.3 The distribution of weak links in narrow lines

If the weak links are long, polygranular segments then the electromigration failures should exhibit at least three corollary features. First, failure should occur preferentially at the longest polygranular segment of the line. Second, the failure sites should be fixed by the microstructure independent of the test conditions, so long as these do not change the basic mechanism of failure. Third, for given test conditions there should be a simple relation between the time to failure and the length of the longest polygranular segment.

One must make a great many observations to establish these points experimentally. It is not practical to do that with high-resolution TEM. However, the TEM observations show that the length of the polygranular segment is almost equal to the separation between the void and the precipitate that are associated with it. The void-precipitate pairs are visible in SEM photographs, and their separations for hundreds of tested lines were measured. The results support three statements.

The weak links are the longest polygranular segments

To determine whether failure occurs at the longest polygranular segment void-precipitate spacings in 275 lines that had been tested to failure were measured. In 234 of these the spacing was largest at the failure site. 25, 10 and 6 lines failed at the second, third, and fourth largest spacings, respectively. None failed at spacings shorter than the fourth largest.

The results are presented in a slightly different form in Fig. 4.21. In this figure the cumulative distributions of void-precipitate spacings at the failure sites (labeled "failed sites" in the figure), and at all observable sites ("damaged sites") for both the 1.3 and the 2 μm lines are presented. In both cases the spacings are larger at the failed sites.

Note that the polygranular segments lengths (as measured by the void-precipitate

Fig. 4.21 The normal distribution of void-precipitate spacings for the failed and damaged sites in unaged 1.3 and 2 μm lines.

spacings) are best fit by a normal distribution, while the distribution of failure times is log-normal (Fig. 4.5). As will be discussed below, this result is in qualitative agreement with simple models proposed by other investigators.

The weak links are fixed by the microstructure

To show that the weak links are fixed by the microstructure investigation was performed to measure the void-precipitate spacings at failed and damaged sites for samples tested at various temperatures, current densities and pre-aging times. Fig. 4.22 shows the mean and standard deviations of the distribution as a function of test temperature. Fig. 4.23 shows similar data as a function of current density. Both statistical measures

are independent of test conditions, in agreement with the hypothesis that the failure sites are fixed by the microstructure.

Fig. 4.24 shows the mean void-precipitate spacing as a function of pre-aging time for the 1.3 μm lines. The data on the two sides of the 24 hr point are connected by a dashed line since the 24 hr specimens failed by a different mechanism. The void-precipitate spacing in the samples that failed by the transgranular-slit mechanism is essentially independent of the pre-aging time. The data are consistent with the hypothesis that the weak links are the polygranular segments. Pre-aging at 226°C does not significantly change the grain size, so the statistical distribution of polygranular segments should remain almost the same. However, pre-aging strongly affects the nature, size and distribution of the Cu-rich precipitates in the line. The data suggest that these changes affect the time required to fail a given polygranular segment. The mean time to failure changes significantly with pre-aging time as shown in Fig. 4.6. Moreover, the density of voids decreases dramatically for intermediate aging times, as shown in Fig. 4.24. Microstructural studies suggest that this is because the shorter polygranular segments in the lines aged for intermediate times do not develop void-precipitate pairs.

The relation between failure time and polygranular segment length

The relation between the polygranular segment length and the time to failure is not given directly by the data described to this point. The tests used samples that contained many lines per specimen, and measured the distribution of failure times without identifying the particular line that failed at each time. However, if we assume that there is a simple relation between the failure time and the polygranular segment length, a relation can be constructed by ordering the measured void-precipitate spacings and the measured failure times, and assuming that the two correspond in inverse order, that is, the

Fig. 4.22 The (A) mean and (B) standard deviation of void-precipitate spacings at damaged and failed sites in 1.3 μm lines tested at various temperatures at $j = 2.5 \times 10^6 \text{ A/cm}^2$.

Fig. 4.23 The (A) mean and (B) standard deviation of void-precipitate spacings at damaged and failed sites in 1.3 μm lines tested at various current densities at 225°C

Fig. 4.24 The mean void-precipitate spacing at failure as a function of pre-aging times for 1.3 μm lines, tested at 225°C and 2.5×10^6 A/cm² after pre-aging at 225°C.

Fig. 4.25 The relation between void-precipitate spacing and failure time for 1.3 and 2 μm lines tested at 225°C and 2.5×10^6 A/cm². The open symbols mark data that was measured by interrupting tests.

longest segment length is associated with the shortest failure time, the second longest with the second shortest, and so on.

This reasoning was applied to the results of tests done on unaged specimens of 1.3 and 2.0 μm linewidths. The results are plotted in Fig. 4.25. To test the validity of the procedure used to obtain Fig. 4.25, additional electromigration studies were performed on unaged 1.3 μm lines in which the test was interrupted for the first four failures and the last three failures, and measured the void-precipitate spacings that were specifically associated with each failure. The results are plotted as open squares in Fig. 4.25. They are in good agreement with the results that were inferred from the original data.

The data fall on straight lines on a semi-log plot, and are, hence, well fitted by a relation of the form

$$t_f = t_0 \exp(-l / l_0) \quad (4.2)$$

where the pre-exponential factor, t_0 , is a characteristic time and l_0 is a characteristic length.

4.3 Electromigration failure in wide lines

The observed failure mode in wide lines was quite similar to the conventional mechanism. Voids nucleate at grain boundaries, and grow along grain boundaries to join one another and break the line. Grain boundary failure in wide lines can be seen from the TEM micrographs shown in Fig. 4.15. Since the failure requires linkage of voids dispersed along grain boundaries, the failure rate is relatively slow. As shown in the resistance variation data (Fig. 4.10), the rate of increase in the resistance for wide lines is much slower than in narrow lines in which one void forms transgranularly and rapidly grows to failure. Also, the critical amount of resistance increase for rapid failure is much higher in wide lines. All of these observations confirm that the failure in wide lines oc

curs through linkage of individual voids in grain boundaries.

In wide lines, the MTF and DTF are slightly dependent on the effective grain size (W/G). The explanation for the MTF and DTF dependence on linewidth is obtainable from the statistical model. As linewidth increases, the line contains more grain junctions with a more uniform distribution, and, hence, it takes more time to break the line through the linkage of voids.

The MTF is improved by pre-aging the line, but the improvement is relatively small. The improvement appears to be due to the growth of precipitates at triple junctions in the aged lines. The most probable position for void nucleation is a triple point of grain junctions [128]. The stable precipitates formed at a triple junction probably act both as a vacancy sink and as a diffusion barrier. Thus they keep triple junctions from voiding until they are dissolved, and leave voids behind by exchanging Cu with vacancies. This is the reason why voids were found at the sites where precipitates were previously located. The role of the precipitates also explains the failure morphology difference between pure Al lines and lines with precipitates. A void at the line edge is the most stable because it requires less energy for void formation and it can lower the stress between the line and substrate. Hence, in pure Al the individual void formed at a triple junction can quickly migrate to the line edge and grow. On the other hand, in lines with precipitates, voids form at the precipitates located at the grain junctions, and are immobile until the precipitates dissolve.

The evidence that the precipitate could act as a diffusion barrier can be seen from the resistance variation of aged lines shown in Fig. 4.11. When the increase in the rate of resistance in aged lines are compared to that in unaged lines, two differences can be noticed. First, the increase rate is slower in aged lines. Second, a sudden decrease of resistance after damage initiation, which physically represents the healing of the damages, frequently appears in aged lines. Once formed, a void should grow with increasing rate

because of the increased current density and temperature at the damaged portion of the line. The healing of the damage means that somehow void growth is counterbalanced by the back flux. A possible mechanism can be found through the concept of a stress gradient induced by electromigration [40-44]. If precipitates act as diffusion barriers, the electromigration flux is blocked at the precipitates until dissolution, and which point the mass accumulates at the precipitates, producing back diffusion. This back-diffusion could heal the damage.

4.4 Electromigration failure in unaged, narrow lines

4.4.1 The metallurgy and statistics of failure in narrow lines

The behavior of unaged, narrow lines can be summarized as follows. Electromigration tests show that the lines fail at times that have a log-normal distribution. Metallographic studies show that failure occurs almost invariably at the upstream termination of the longest polygranular segment in the line, irrespective of test conditions. The longest polygranular segments, as measured by the maximum void-precipitate spacings, have a normal distribution.

The correlation between segment lengths and failure times presented in Fig. 12 suggests that the two are exponentially related according to eq. (4.2). These results are internally consistent. If the segment lengths and failure times are related by eq. (4.2), a normal distribution of maximum segment lengths will produce a log-normal distribution of failure times.

4.4.2 The failure mechanism

The failure mechanism that governs the life of unaged, narrow lines is the trans

granular-slit failure mode, which was also observed by others [97, 129-131]. A notch appears in the edge of the line and propagates across a bamboo grain to cause failure. The observations made here show that this almost always happens first in the bamboo grain that terminates the longest polygranular segment in the line.

While several key features of this mechanism are not yet understood, it seems clear that the failure results from a supersaturation of vacancies injected into the grain from the polygranular segment. A likely mechanism is the condensation of supersaturated vacancies that forms the original notch, which grows across the grain to cause failure in a dendritic growth pattern. Mechanical stresses in the line may also play a role. The thermal mismatch between the line and the substrate is a one source of mechanical stress. In addition, accumulated vacancies can introduce tensile stress into the bamboo grain. Nucleation of voids along the edge of the line is favored because nucleation at this site relaxes the mismatch stress. Vacancies should preferentially condense on the crystallographic plane where the surface energy is the lowest. In aluminum, (111) planes provide such sites. Hence, the edge void is faceted along close-packed planes, forming a notch. At the head of the notch, the vacancy condensation becomes substantial due to a reduced dimension, and the void grows dendritically through the condensation of vacancies on (111) planes. Rose [129] reported that the transgranular silt voids in passivated Al-2Cu interconnects were aligned along the $\langle 110 \rangle$ direction with faces parallel to (111) plane. Sanchez et al. [131] also found the similar relation in unpassivated Al and Al-2Cu interconnects. It seems that the crystallographic orientation of the grain that fails to the surface normal would determine the direction of the slit void. It is also possible that the lines are actually fractured at the last stage of the void growth. It is not possible to describe the mechanism in detail, but prior work does suggest the source of the vacancy supersaturation and the reason that it is most pronounced at the head of the longest polygranular segment.

In agreement with these observations, the activation energy for failure for the transgranular failure observed in narrow lines is near 1.0 eV, which is near the activation energy for bulk diffusion in Al-Cu [31, 34], while the activation energy for intergranular failure in wide lines is near 0.6 eV, a plausible value for grain boundary diffusion [35-38].

Fig. 4.26 Schematic representation of single grain boundary terminated by a bamboo grain, running parallel to the line direction.

4.4.3 The diffusion model

Various theoretical models have been used to predict the accumulation of vacancies during electromigration. The simplest are grain boundary diffusion models, such as that proposed by Arzt and Nix [134], and developed by Lloyd [95], and Kirchheim and Kaeber [135], which compute the vacancy enrichment at the head of a grain boundary due to the high vacancy diffusivity along the boundary. The second set of models considers the stress developed by the accumulation of vacancies at a flux divergence, and calculates the vacancy concentration due to the balance between electromigration and stress-induced back-diffusion [68-72]. The two models lead to qualitatively similar relations.

First consider the diffusion model. The diffusion model simulates the vacancy accumulation at the end of a grain boundary of length, l , that is oriented parallel to the cur-

rent flow, as schematically presented in Fig. 4.26. Because of the blocky grains at both ends of the grain boundary, it can be approximated that the fluxes at these ends are zero:

$$J_v(x=0) = J_v(x=l) = 0 \quad (4.3)$$

The diffusion equation of vacancies in this grain boundary is given as

$$\frac{dC}{dt} = -D \frac{d^2C}{dx^2} + v \frac{dC}{dx} \quad (4.4)$$

where D and v represent the grain boundary diffusivity and the drift velocity of vacancies, respectively. The drift velocity of a vacancy, v , is defined as

$$v = \frac{D}{kT} eZ^*E \quad (4.5)$$

where Z^* denotes the effective valence of vacancies at grain boundaries, which is presumably the same as that of Al atoms. Using the boundary condition in eq. (4.3), eq. (4.4) can be solved, and the solution yields an infinite series of eigenfunctions and an exponential time function, where the largest among the corresponding time constants determines the time for the attainment of a stationary concentration profile [135]:

$$C(x,t) = A \exp\left(\frac{vx}{D}\right) \left[1 + B(x) \exp\left(-\frac{t}{\tau_c}\right)\right] \quad (4.6)$$

where A and $B(x)$ have to be calculated from the initial condition and τ_c is the largest time constant for obtaining a steady state concentration profile. In this model the sink and source terms for the vacancies (in which case the average lifetime of vacancies should be included as in eq. (1.33)) are not considered because the results are qualitatively the same as eq. (4.6). At a steady state condition, Arzt and Nix, and Lloyd showed that the vacancy concentration at position l satisfies the relation

$$C(l) = C_0 \exp\left(\frac{vl}{D}\right) \quad (4.7)$$

where C_0 is the equilibrium vacancy concentration in the absence of current. If we as

sume that the time to failure is inversely proportional to the vacancy concentration at l , which determines the rate at which vacancies are injected into a bamboo grain located beyond the boundary, this model predicts a relation of the form (4.2),

$$t_f = t_o \exp\left(-\frac{l}{l_o}\right) \quad (4.8)$$

where t_o is the time to failure in the absence of a grain boundary, and the effective length,

$$l_o = \frac{D}{v} = \frac{kT}{Z^* e E} \quad (4.9)$$

is determined by the ratio between the temperature, which tends to randomize the distribution of vacancies, and the force imposed by the electric field, which drives them in a particular direction. The effective length at 225°C under current density of 2.5×10^6 A/cm² is approximately 4 μ m, taking $Z^* \sim 10$ and resistivity $\rho \sim 5 \times 10^{-6}$ Ω -cm [135].

The qualitative explanation for the failure at the longest segment length can also be obtained using the concept of an electromigration-induced stress gradient, as discussed earlier. Since the electromigration along the grain shown in Fig. 4.26 is much faster than through the bamboo grains, mass will accumulate at the position $x = 0$ and mass will be depleted at the position $x = l$. As derived in eq. (1.35), the electromigration flux at the grain boundary is inversely proportional to the grain boundary length l :

$$J = J_{l=\infty} \left(1 - \frac{l_c}{l}\right) \quad (4.10)$$

where l_c denotes the critical length beyond which no electromigration occurs, the so called Blech length. If we assume that the lifetime is inversely proportional to the electromigration flux J , it can be seen that the longer l shows the shorter lifetime, although the exponential variation of lifetime with the length is not achieved as the diffusion model.

Both the diffusion model and the stress gradient model provide at least qualitative descriptions of grain boundary length dependence of lifetime. However, we can not ex-

clude either one of these two possibilities from the plausible mechanism. If we take both mechanisms together by writing the diffusion equation of vacancies as

$$\frac{dC}{dt} = -D \frac{d^2C}{dx^2} + v \frac{dC}{dx} - \frac{\Omega d\sigma}{dx} \quad (4.11)$$

where the last term represents the influence of stress gradient on the vacancy diffusion, and is defined in eq. (1.26). Applying the same calculation as eqs. (4.3)-(4.7), the vacancy concentration at $x = l$ can be obtained, and has the simplified form

$$C(l) = C_o \exp\left[\frac{l}{l_o} \left(1 - \frac{l_c}{l}\right)\right] \quad (4.12)$$

Then one obtains the lifetime as

$$t_f = t_o \exp\left[\frac{l}{l_o} \left(1 - \frac{l_c}{l}\right)\right] \quad (4.13)$$

When the influence from the stress gradient is relatively small, eq. (4.13) becomes eq. (4.8), the case when the current density is relatively high. This prediction can be explained as follows. The stress gradient term used in eq. (4.11) is derived when the stress gradient is fully developed. In the actual case, however, the development of stress gradient is time dependent. The time to reach to the diffusional steady state condition of a vacancy profile should be much faster than that of the stress gradient build-up. Hence, if failure occurs without inducing much of a stress gradient, as when testing under high current densities, the effect from the stress gradient must be small enough to be ignored. The current density used in this study can be considered to be high enough to ignore the stress gradient effect. It is believed, however, that the stress gradient influences the failure kinetics, although that influence is still insignificant. In Fig. 4.10, it was noted that there exists a healing of damages for a short amount of time in some cases. The l_c is expected to be sensitive to the formation of transgranular void. While overall stress gradient is not changed by void formation, local stress where the void is formed should be significantly changed, which may increase l_c . When l_c becomes comparable to or greater

than the grain boundary length l , the vacancies move backward and lower vacancy concentration below the equilibrium value, which means that voids are healed. This explanation might be too primitive to account for the healing mechanism during electromigration and requires more investigation. Healing even after complete failure frequently observed in narrow lines, however, leads to the belief that the stress gradient plays a role in the healing process.

The model introduced here is too simple to give an accurate analysis of the vacancy distribution across a polygranular segment that may contain several grain boundaries with junction lines and various orientations, and it does not explain the effects of linewidth or precipitate distribution. However, it does have the correct qualitative behavior. It predicts that failure occurs at the longest polygranular segment, and that the failure time is inversely proportional to the exponential of the segment length.

4.4.4 The influence of linewidth

We confine our attention to lines that are narrow in the sense that they have partial bamboo structures and fail by the transgranular-slit mechanism. For these lines, both the median time to failure and its standard deviation decrease as the linewidth increases with respect to the mean grain size (i.e., as W/G increases). A first-order explanation of these changes follows from the association between failure time and polygranular segment length. If two lines of equal length are patterned from films that have the same statistical distribution of grain sizes, then the wider line is likely to contain a longer polygranular segment, and the fractional deviation from the mean value of the longest segment length is likely to be smaller. However, if this were the whole explanation then the values of t_0 and l_0 in eq. (4.8) would be independent of linewidth. The data in Fig. 25 show that they are not; t_0 is smaller and l_0 is larger for the wider lines.

The factor, t_0 , in eq. (4.8) is the extrapolated failure time for a line with $l = 0$, that is, for a line that has a completely bamboo structure. There are good reasons to expect that the time to failure of a bamboo line decreases with its width. The vacancy supersaturation that leads to transgranular failure can be relieved by diffusion to free surfaces. Hence the degree of supersaturation that is developed under given conditions should decrease with the surface-to-volume ratio of the line. This effect was explored in work by Kwok and others [65, 136], who studied the influence of line thickness on the lifetime of Al alloy lines. They found that lifetime increased as film thickness decreased. Assuming that this result is due to vacancy diffusion to the free surfaces, decreasing width at constant thickness should have the same effect.

The diffusion model suggests that the factor, l_0 , in eq. (4.8) measures the balance between the unidirectional vacancy flow caused by the field and the back-flow due to thermal homogenization. The characteristic length, l_0 , increases as the electrical factor becomes less important with respect to the thermal one. While the polygranular sections are longer in a wide line, the grain boundaries within them should be, statistically, more complex in their arrangement and more angled with respect to the axis of the line. Both of these factors may decrease the response to the electric field, and, hence, increase l_0 . It may also be possible that the failure kinetics in wider lines is slower than in narrower lines because a nucleated void has to travel a longer distance across the width in wider lines, provided that the critical size of a stable void is the same.

4.5 The influence of Cu and the effect of pre-aging

4.5.1 The role of Cu

One of the most interesting results to emerge from this work is the observation that Cu precipitates are swept from both the polygranular segment and the bamboo grain that eventually fails before final failure. This observation suggests a role of Cu in the

failure mechanism and helps to explain the dramatic effect of pre-aging on the mean time to failure.

It is well known from prior work [14, 15, 18, 19] that Cu associates with vacancies in Al-Cu alloys and exchanges preferentially with them in an electric current. Because grain boundaries offer easy diffusion paths, the polygranular segments in a narrow line have a higher net diffusivity than the bamboo grains. It is, hence, not surprising that Cu should be swept out of the polygranular segments. Cu moves with the current, and should accumulate in the bamboo grain at the downstream side of the segment, where the diffusivity decreases discontinuously. The large, Cu-rich precipitate at the downstream side of the segment apparently forms as a consequence of this accumulation and provides an effective sink for Cu [137].

As Cu diffuses downstream, vacancies migrate upstream. The vacancy concentration at the head of the polygranular segment produces a concentration gradient that drives vacancies into the bamboo grain and enhances Cu diffusion out of it. The result is to sweep Cu from both the polygranular segment and the grain upstream. Since Cu exchanges preferentially with vacancies, its presence increases the bulk diffusivity of the vacancies [19]. This enhanced bulk diffusion combines with diffusion to free surfaces to reduce the supersaturation of vacancies near the boundary of the polygranular segment. However, when Cu is depleted the vacancy diffusivity in the bulk decreases significantly. The vacancy supersaturation increases, and, apparently, reaches a critical value at which vacancies condense into edge voids that grow to failure.

4.5.2 The effect of pre-aging

If this analysis is correct, Cu retards electromigration failure in narrow lines by increasing the rate of diffusion of vacancies through the bulk. Failure occurs rapidly once the Cu is swept away. Assuming that there is much more Cu present in an Al-2Cu line

than is needed to accomplish this, the time to failure will be increased by any change in the internal state of the Cu that increases the time required to sweep it away. In unaged, rapidly cooled lines, Cu is present in GP zones that are high-energy precipitates. As the line is aged, these form into larger, metastable θ' precipitates, which then transform into relatively stable θ precipitates. Overaging causes these to dissolve in favor of θ -phase precipitates in the grain boundaries.

Fig. 4.27 A comparison between the MTF and the precipitate type and density as a function of pre-aging time for 1.3 μm lines aged and tested at 225°C and 2.5×10^6 A/cm².

The longest-lived Cu precipitates should be θ -phase precipitates in the grain interiors. Since θ is thermodynamically stable with respect to θ' or GP zones, the chemical resistance to dissolution by the current is higher. θ -phase precipitates in grain boundaries are still more stable, but the ease of diffusion along grain boundaries causes them to dis-

solve more rapidly. The time to failure increases dramatically as GP zones are replaced by θ' precipitates and then by intragranular θ precipitates. It falls as the intragranular θ coarsens into the grain boundaries. The dependence of the MTF on the density of intragranular θ precipitates is shown in Fig. 4.27. This figure is a composite plot of Fig. 3.9 and Fig. 4.6, which compares the MTF and the intragranular precipitate density as functions of aging time. The MTF increases and decreases in parallel with the intragranular density of θ , but is relatively unaffected by θ' .

When the aging temperature is raised, the maximum attainable density of intragranular θ is lower, and is reached at shorter aging times, because of accelerated coarsening in the grain boundaries. The test results with the variation of aging temperatures show that increasing the aging temperature to 310 °C decreases the maximum in the MTF by 40% and displaces it toward shorter aging times (Fig. 4.8). On the other hand, aging at a lower temperature, 190°C, for 48 hours is not enough to develop the maximum density of intragranular θ because of slower kinetics of precipitation, the MTF increase slowly without a peak.

In the optimally aged condition the mechanism of failure changes from the transgranular-slit mechanism discussed here to a diffuse thinning mechanism in which the bamboo grain at the upstream terminus of the longest polygranular segment gradually thins until it finally ruptures. The probable explanation for this failure mechanism is that the Cu retained within the grain is sufficient to prevent the development of a supersaturation that is great enough to cause slit failure. The excess vacancies that are injected into the grain from the polygranular segment diffuse to the free surfaces of the bamboo grain and annihilate there, resulting in a gradual thinning of the line. This diffuse thinning eventually leads to rupture. Hence the failure rate of the diffuse thinning mechanism as measured by the resistance change is slow and steady, as shown in Fig. 4.11.

The amount of excess vacancies injected into bamboo grains depends on the

polygranular segment length. Hence, the lifetime of the diffuse thinning failure is also sensitive to the linewidth in a sense that the wider line contains longer polygranular segment. This provides the explanation for the strong linewidth dependence of MTF on the effective linewidth (W/G) of optimally aged samples (Fig. 4.7).

Pre-aging has another important consequence. As shown in Fig. 4.5, the shortest failure times in pre-aged lines are much longer than predicted by the log-normal distribution. Approximately the first 25% of failures in optimally pre-aged lines occur at nearly the same time. This retardation of the first failure has important practical consequences since devices must ordinarily be designed to avoid the first failure of a conducting line. Since the first failures occur at the longest polygranular segments, these results suggest that the time required to sweep Cu from long polygranular segments in properly aged lines is relatively insensitive to segment length when the length exceeds some critical value. The mechanism of this preferred enhancement is explored in the next chapter.

4.6 Summary

The results presented here reveal that the failure mechanism is influenced by the linewidth and the stability of Cu. In wide lines, the failure occurs through void nucleation and growth along grain boundaries, which is the same as the conventional failure mechanism. Precipitates at the grain boundaries retard void formation and, accordingly, the lifetime slowly increases with the pre-aging time due to the stabilization of precipitates.

In narrow lines, failure occurs through bamboo grain rather than at grain boundaries. The transgranular failure mechanism that governs the life of narrow Al-Cu-Si conducting lines is due to the accumulation of a supersaturation of vacancies in the bamboo grains that terminate polygranular segments in the line. Under the conditions tested here,

failure occurs after Cu has been swept from the grain that fails. For a given distribution of Cu, failure happens first at the end of the longest polygranular segment of the line, at a time that decreases exponentially with the polygranular segment length. Pre-aging the line to create a more stable distribution of Cu within the bamboo grains lengthens the time required to sweep the Cu from the longest polygranular segment, and significantly increases the time to failure. In the optimal case the transgranular-slit failure mechanism is suppressed, and the bamboo grain fails by diffuse thinning to rupture. Pre-aging is particularly effective in increasing the lifetimes of lines that contain very long polygranular segments, and has the consequence that the time to first failure in an array of lines is much longer than predicted by a log-normal fit to the distribution of failure times.

The results suggest that a processing technique that effectively eliminates long polygranular segments from narrow lines will produce an exponential increase in life. An additional dramatic improvement can be made by aging or otherwise processing the lines to develop a stable distribution of intragranular precipitates. Pre-aging is particularly effective in increasing the life of lines that contain long polygranular segments, and hence provides an added margin of safety against early failures.

CHAPTER 5

ELECTROMIGRATION OF PRECIPITATES

The microstructural study of the failure mechanism described in chapter 4 revealed that the addition of Cu enhances the electromigration lifetime by increasing amount of Cu-rich precipitates, which may act as a vacancy sinks, diffusion barriers and reservoirs of Cu that enhance the diffusivity of vacancies. The remaining question is how electromigration force influences the degree by which these precipitates play such roles. In order to answer this question, it is essential to understand the mechanism of precipitation and dissolution during electromigration. For this purpose, a simple experiment was designed. Before applying a normal current in which the direction of current is the same as in the previous studies, an equal current with reversed polarity was applied for various times. As seen in the failure mode in narrow lines, Cu preferentially migrates in the direction of electron flow, resulting in the unique feature of a void-precipitate pair. During initial current stressing with reversed polarity, it is plausible to assume that the void-precipitate pair appears with the opposite polarity of the normal case. Then, when the current polarity is changed to the normal direction before the line fails, the polarity of the void-precipitate pair may be or may not be reversed, depending on the interaction of the electromigration force and the precipitate. The answer to this question will lead to a key understanding of the role of precipitates in electromigration failure.

The study on current reversal was done using samples deposited under the planarizing condition, which allows a comparison of the failure mechanism with the results presented in the previous chapter. Through an analysis of the test results, it was established that the precipitate actively interacts with the electromigration force. In addition,

the preferred enhancement of the first few failures in aged, narrow lines was explained.

5.1 Failure as a function of current-reversal time

The lifetime of the test lines were measured as a function of current reversal time, τ_R , during which the polarity of the current was reversed. This test was performed under the same conditions as most of the other tests: a substrate temperature of 225°C and a current density of 2.5×10^6 A/cm². As can be seen in Fig. 5.1, the net time to failure physically measures the failure time by the current only with the normal polarity. The test results are compared in Figs. 5.2-5.5.

Fig. 5.1 A schematic illustration of a current reversal test. The polarity of current direction is changed after reversal time τ_R .

The mean of the net time to failure (MNTF) for different linewidths as a function of τ_R is summarized in Fig. 5.2. For 1.3 and 2 μm lines, MNTF initially increases by about a factor of two and then decreases as τ_R increases, while for wide lines there is either no significant change (4 μm) or a slight increase (6 μm) in the MNTF. It appears that the peak τ_R depends on linewidth; MNTF is a maximum when τ_R is 2 hours for 1.3 μm and 3 hours for 2 μm .

As can be seen from the failure statistics shown in Figs. 5.3-5.5, the effect of current reversal is not uniform but affects the first few failures more profoundly. For narrow

Fig. 5.2 (A) MNTF and (B) relative MNTF as a function of current reversing time, τ_R , for unaged lines of four line widths.

Fig. 5.3 A log-normal plot of net time to failures for unaged, 1.3 μm lines for various current reversing times.

Fig. 5.4 A log-normal plot of net time to failures for unaged, 2 μm lines for various current reversing times.

Fig. 5.5 A log-normal plot of net time to failures for unaged, 6 μm lines for various current reversal times.

lines, the increase in the low percent failure time is especially substantial, resulting in a bimodal distribution of lifetimes. When 1.3 and 2 μm lines are compared, a bimodal distribution of lifetime is more significant in the 2 μm lines.

As τ_R increases, the beneficial effect from current reversal decreases. The decrease is more rapid in long-term failures than the short term failures, except for the first 2 failures after current reversal in 1.3 μm lines. The first two failures after current reversal found in 1.3 μm lines shows almost the same net time to failure as lines with no current reversal.

5.2 Microstructural failure mechanism with current reversal

The morphological feature of failure sites with current reversal was studied under

SEM. This study revealed that the microstructural failure mechanism of lines with current reversal is basically the same as that of lines without current reversal. For wide lines, failure is followed by the nucleation and coalescence of voids along grain boundaries, irrespective of reversal time.

The failure sites found in 1.3 μm lines are summarized in Fig. 5.6 as a function of τ_R . For any τ_R , almost all of the failure sites contain a void-precipitate pair, and the polarity of the pair is the same as in the lines without current reversal. However, there is a qualitative variation of the failure morphology with current reversal. As τ_R increases up to 2 hours, at which the net time to failure is maximum, the failure morphology is exactly the same as in lines without current reversal (Fig. 5.6.A, B), i.e., a large θ precipitate is located on the down stream side of the transgranular slit-void. When τ_R is increased further, some of the failed voids appear to extend to an adjacent grain boundary, resulting in relatively larger voids, while the polarity of the void and θ -phase precipitate is maintained (Fig. 5.6.C-E). In some cases, a second void appears in the middle of the void-precipitate pair (Fig. 5.6.D). This second void, however, does not grow to failure. When τ_R is 4 hours, there are 3 other distinctive failure modes in addition to the normal failure mode. The first failure mode takes place in lines failed during current reversal. The first 4 lines failed during current reversal. In this case, the polarity of the void-precipitate pair is opposite to the relative others, as expected. The second failure mechanism is shown in Fig. 5.6.G; the polarity of the pair is the same as in the failure during current reversal. However, the void and the θ precipitate are located adjacent to each other. Two lines failed with this mode. Finally, two failure sites were found to be a combination of the normal failure mode and the second failure mode described above. As shown in Fig. 5.6.F, a precipitate appears at a void with reserved polarity, while the other void is visible on the downstream side. The failure mode found in the 2 μm lines is the same as the 1.3 μm lines described here, except for the absence of the second failure morphology.

Fig. 5.6 SEM micrographs showing failure mode evolution in 1.3 μm lines with current reversal time: (A-B) $\tau_R = 2$, (C-E) $\tau_R = 3$, and (F-H) $\tau_R = 4$ hours. (XBB 933-1213)

5.3. Kinetics of Failure with current reversal

If void formation and growth are the only requirements for failure, the net time to fail the lines should qualitatively be the same or less for any τ_R ; this is especially true for pure Al. However, if any reversible damage produced during current reversal is healed before failure, it takes a longer net time for failure occur [138]. For wide lines, there was a slight gain in time to failure by current reversal. During current reversal, precipitates at triple junctions, where the flux diverges, dissolve and voids form by exchanging Cu with vacancies, while precipitates at flux convergence points preferentially grow. When the current direction is changed, the flux divergence condition at these points would be reversed. Hence, it takes a longer time to dissolve the enriched precipitates, resulting in an enhancement in the net time to failure (6 μm lines). This effect is, however, relatively small.

The influence of the precipitate has a greater impact on the net time to failure in the narrow lines. The time to failure (t_f) of unaged, narrow lines can be considered as a sum of the time to sweep Cu in a polygranular segment (t_p), in a bamboo grain (t_b) and the time to form and grow a void (t_v):

$$t_f = t_p + t_b + t_v \quad (5.1)$$

Depending on the relative importance of these time factors, the time to failure will be determined. From the lifetime results of pre-aged lines, it was determined that t_b is the key factor which determines the time to failure. However, the contribution of t_p can not be ignored, even though it is small.

During current reversal, it is likely that the precipitate at a polygranular segment is swept in the direction of mass flow, forming a large θ precipitate at the downstream side of the segment. When τ_R is short, the sweeping of Cu and subsequent void formation would not progress. When the direction of current is changed, the θ precipitate is

placed on the upstream side of the mass flux and, hence, it must be swept to downstream side again. In this case, a longer time is required to sweep Cu in a polygranular segment than before since Cu atoms are stabilized in the form of a downstream side precipitate. This process is schematically represented in Fig. 5.7.A. Hence, the net time to failure increases with increasing τ_R .

There are counterbalancing effects, however, when the current reversal time is longer than optimum. During reversed current, the bamboo grains located at the upstream side loses Cu to θ precipitates formed at near grain boundaries (Fig. 5.7.A.a). Hence, the sweeping rate of Cu at this grain under the normal current direction would be faster than before. The sweeping of Cu in the polygranular segment is also faster. When the triple points in a polygranular segment are decorated with precipitates, which form in spite of electromigration until all the Cu in adjacent grains are consumed, the migration rate of Cu is slower than a single, big precipitate without a supply of Cu (Fig. 5.7.B). The net time to failure, thus, decreases due to a decrease in t_b and t_p after the optimum τ_R . It appears that when a single, large θ precipitate dissolves and migrates, there is a tendency to form a void at the site, which might account for the extension of voids to the grain boundary observed in some cases (Fig. 5.7.B.b).

In extreme cases when there exists a stable void induced during the reversed current, this void grows and causes failures even under normal current (Fig. 5.6.G). Since this void grows only by self-induced flux divergence, its growth rate is relatively slow, competing with the tendency to form a void at the other end of the bamboo grains in which vacancies are coming from the polygranular segment. If this existing void grows before another void forms at the normal site, the failure site will contain the void-precipitate pair placed adjacent to each other with reversed polarity. If the formation and growth of a void at a normal site is faster than the existing void, the subsequent failure site has the feature that is combination of the two failure processes (Fig. 5.6.F). These failure mechanism are presented schematically in Fig. 5.8.

Fig. 5.7 Schematic representation of failure mechanism when (A) τ_R is less than the peak τ_R and (B) τ_R is longer than the peak τ_R .

Fig. 5.8 Schematic representations of failure mode comparing the case when failure occurs (A) at pre-existing void formed during current reversal and (B) at a normal void developed after current reversal.

The sweeping kinetics of precipitates in polygranular segments depends on the segment length: it takes a longer time to sweep a Cu precipitate from longer segment. Hence, for a given width, the net time to failure is greater in a longer segment, causing a bimodal distribution in the failure statistics. The lengths of the polygranular segments in wide lines are longer than in narrow lines, thus, producing a greater bimodal distribution in the failure statistics. In addition to this, since polygranular segments in wider lines contain more triple junctions where precipitates form, the sweeping of Cu is slower, increasing the time to sweep the Cu precipitate that had migrated during current reversal; the peak τ_R is longer in wider lines.

5.4 Effect of t_p on failure time of pre-aged lines

Through above observations, it has been established that the time to sweep Cu in a polygranular segment, t_p , has some contribution on the time to failure, t_f , but not significantly; the net time to failure by current reversal increased by a factor of two at most. On the other hand, pre-aging of lines can increase the lifetime by more than an order of magnitude. In unaged lines, it seems that the contribution of t_p on t_f is about the same as that of t_b and t_v ; they are comparable, and, thus, lifetime statistics are close to monomodal. As lines are pre-aged, the θ precipitates start to decorate both the bamboo grains and the triple points in polygranular segments. Hence, contribution from t_p and t_b on t_f increases accordingly while t_v should be independent of pre-aging, unless the failure mechanism changes to diffuse thinning. It seems that the increase in t_b is more rapid than in t_p as it was found that the MTF rapidly decreases with linewidth in the optimum aging condition (Fig. 4.7). Therefore, the MTF rapidly increases with pre-aging from t_b , while t_p has a slight but beneficial effect on the time to failure of first few failures, resulting in a bimodal distribution of lifetime statistics.

5.5 The role of precipitates

Through the current reversal test, it is shown that the precipitate is indeed dissolved by electromigration, regardless of its initial stability. Also, the electromigration lifetime depends on the sweeping rate of the precipitates. The detailed mechanism of the precipitate dissolution and electromigration is still unknown and requires deeper investigation. However, a simple and qualitative mechanism may be suggested as an initial approach. As a start, it would be informative to describe the mechanism of natural coarsening, so that the analysis can be expanded to the precipitate coarsening under electromigration force. The coarsening mechanism discussed here assumes that the migration of solute atoms is the rate-limiting reaction of the precipitate dissolution.

Fig. 5.9 A schematic representation of the concentration gradient of Al and Cu atoms across the precipitates; Cu atoms migrate to the larger precipitate, while Al atoms migrate in the opposite direction.

5.5.1 The mechanism of precipitate coarsening

Consider the two equilibrium Al_2Cu -phase precipitates of different radii located adjacent to one another. In this case, a larger precipitate tends to grow by taking Cu from the smaller precipitate, which will eventually disappear [139, 140]. The migration of Cu

to the larger precipitate occurs due to the chemical potential gradient existing across the precipitates. The chemical potential gradient comes from the concentration difference of solute atoms at the matrix around each precipitate. This precipitate size effect on the concentration is known as the Gibbs-Thomson effect: the concentration of Cu around the smaller precipitate is higher than around the larger precipitate and it increases exponentially with decreasing size [139]. Therefore, the driving force becomes greater as the coarsening proceeds further because of the exponential increase in the concentration gradient. This is the conventional description of precipitate coarsening.

During the coarsening process, it should be noted that the diffusion of Cu atoms induces the diffusion of Al atoms. The concentration gradient of Cu should develop a concentration gradient of Al atoms which drives the Al atoms to move in the opposite direction. The development of a concentration gradient across the precipitates is schematically illustrated in Fig. 5.9. The growing precipitate must give away Al atoms to form more Al_2Cu , while the Al_2Cu in the dissolving precipitate must be replaced with Al atoms. Therefore, the growing precipitate acts as a source of Al atoms, while the dissolving precipitate acts as a sink of Al atoms. The movement of Cu and Al atoms in this case is quite similar to that of an interdiffusion experiment [141].

If we consider the coarsening process as an interdiffusion of Al and Cu atoms, the diffusion flux of each element can be phenomenologically expressed, although the situation of interdiffusion is not exactly the same as the coarsening process in a sense that interdiffusion is not involved with the source and sink as in the coarsening case. For simplicity, denote Al as solvent a and Cu as solute b . Assume that the concentration of Cu at each precipitate is time independent, which is true only during the middle of coarsening. Although the concentration gradient increases with coarsening, the transition of the concentration gradient is not considered here. From eq. (1.13) and the Gibbs-Duhem equation [16], the atomic flux of Al (labeled as " a ") and Cu (" b ") in a lattice frame can be rep

resented as

$$\begin{aligned}
 J_a &= -kT[L_{aa}\frac{\nabla C_a}{C_a} + L_{ab}\frac{\nabla C_b}{C_b}] \\
 J_b &= -kT[L_{ab}\frac{\nabla C_a}{C_a} + L_{bb}\frac{\nabla C_b}{C_b}] \\
 J_v &= -(J_a + J_b)
 \end{aligned} \tag{5.2}$$

where the definition of L_{aa} and L_{bb} can be found in eq. (1.15). Using the relations in eq. (1.17), and $\nabla C_a = -\nabla C_b$, eq. (5.2) can be reduced to

$$\begin{aligned}
 J_a &= D_a \nabla C_b \\
 J_b &= -D_b \nabla C_b \\
 J_v &= -(D_a - D_b) \nabla C_b
 \end{aligned} \tag{5.3}$$

where D_a and D_b physically represent the correlated diffusivity of a and b atoms. Although D_a and D_b is higher than the uncorrelated diffusivity of a and b atoms because of the negative vacancy-flow effect in Al-Cu alloys, $L_{ab}/L_{bb} < 0$ [19], the resulting difference is almost negligible because of its small contribution. In eq. (5.3) the atomic flux of a atoms is represented in terms of the concentration gradient of b atoms, so that the diffusion direction of a atoms is opposite to the b atoms.

As expected, the net flux of a and b atoms generates the diffusion flux of vacancies, and the magnitude of the vacancy flux is determined by the difference in the diffusivity. It is expected that the direction of vacancy flux is the same as that of the b atoms when $D_a > D_b$, while the opposite is true when $D_a < D_b$. For the lattice diffusion in Al-Cu alloys, D_a is higher than D_b for two reasons. First, the self-diffusivity of Al is slightly faster than the correlated diffusivity of Cu, i.e., $D_b/D_a(0) = 0.86$, where $D_a(0)$ represents the self diffusivity of Al atoms in pure Al [19]. Second, the diffusivity of Al is enhanced by Cu because of diffusivity enhancement from the presence of Cu atom. The diffusivity enhancement factor of Cu to Al diffusion is about 100 [19], so that

$$D_a = D_a(0)(1 + b' C) = D_a(0)(1 + 100C) \tag{5.4}$$

where b' denotes the enhancement factor. Therefore, the vacancy flux should move with Cu atoms, i.e., to the growing precipitate. Although these vacancies tend to form a void at the growing precipitate, known as a Kirkendall void, they would be annihilated by the presence of an Al source. On the contrary, if a vacancy moves toward a dissolving precipitate, i.e., $D_a < D_b$, Kirkendall voids would form at the site where the precipitate was previously located.

Kirkendall voids were not found either in the matrix or at the grain boundaries in the course of natural coarsening. For the case of coarsening in the matrix, the absence of Kirkendall voids is an expected result. Since the grain boundary diffusivity of Al and Cu atoms is not available, the analysis can not be completed for the grain boundary precipitate. However, the absence of Kirkendall voids at the grain boundaries suggests that the relative magnitude of grain boundary diffusivity of Al and Cu atoms is either comparable or similar to that in the lattice diffusion case.

5.5.2 Precipitate coarsening under electromigration

The electromigration force imposes the directionality of flow on both solvent and solute migration. It can be assumed that the initial distribution of precipitates is rather random, and primarily located at triple grain junctions. The migration of Cu is then biased by the electromigration force. During the transient stage, it is likely that the precipitates in the flux convergence points are forced to grow, while the precipitates at the flux divergence points are forced to dissolve. The precipitate coarsening situation shown in Fig. 5.9 will be developed after an initial transition stage.

Precipitate coarsening is driven by both the chemical potential and the electromigration force. These two forces induce different kinetics from the natural coarsening process. Under the electromigration force, the phenomenological equation of atomic flux of a and b atoms can be obtained from eq. (1.13) and eq. (5.2):

$$\begin{aligned}
J_a &= D_a \nabla C_b + \frac{D_a Z_a^{**} e E}{kT} C_a \\
J_b &= -D_b \nabla C_b + \frac{D_b Z_b^{**} e E}{kT} C_b
\end{aligned}
\tag{5.5}$$

in which Z_a^{**} and Z_b^{**} are the apparent effective charges under the influence of the vacancy flow effect (eq. (1.19)). Again, the vacancy flow effect on the diffusivity can be assumed to be small. Eq. (5.5) indicates that the total flux of a atom is the difference of the electromigration flux and the diffusion flux. On the other hand, the total flux of b atoms is the sum of the electromigration and the diffusion flux. The interaction of the electromigration force and the diffusion force can be visualized through a simple example. If we assume that the concentration gradient across the precipitates is linear, then eq. (5.5) becomes

$$\begin{aligned}
J_a &= D_a \left[\frac{\Delta C_b}{l_p} - \frac{C_a}{l_o^a} \left(1 + \frac{L_{ab}}{L_{bb}} \frac{D_b}{D_a} \frac{Z_b^*}{Z_a^*} \frac{C_b}{C_a} \right) \right] \\
J_b &= -D_b \left[\frac{\Delta C_b}{l_p} + \frac{C_b}{l_o^b} \left(1 + \frac{L_{ab}}{L_{bb}} \frac{Z_a^*}{Z_b^*} \right) \right]
\end{aligned}
\tag{5.6}$$

in which l_p represents the spacing between precipitates, and l_o 's are the effective length of electromigration defined as

$$l_o^a = \frac{kT}{Z_a^* e E}, \text{ and } l_o^b = \frac{kT}{Z_b^* e E}
\tag{5.7}$$

In these equations, the direction of the electromigration force is chosen toward the negative direction, so that the electromigration force is causing coarsening of the precipitates. Again, it becomes clear that the electromigration of an a atom must overcome the diffusion flux, while the migration of an b atom is enhanced by electromigration.

During coarsening, the Cu concentration within a growing precipitates is close to the solubility limit, while that at a dissolving precipitate can be significantly higher. Since the cutoff concentration at which the precipitate is completely dissolved is unknown, the concentration gradient can not be given. We can assume that the time-aver-

age of the concentration at the dissolving precipitate is 5 times higher than the solubility limit, for example. Since the precipitates in thin films are primarily located at the triple points, we can take $0.5 \mu\text{m}$ for l_p . Then from eq. (5.6), the induced concentration gradient for Al atoms corresponds to $l_o = 100 \mu\text{m}$ when the solubility limit is 0.1%. This length is equivalent to a current density on the order of 10^5A/cm^2 according to eq. (5.7), taking $\rho = 5 \times 10^{-6} \Omega\text{-cm}$, $Z_{\text{Al}}^* \sim -10$ for the grain boundary [39, 40, 135, 142, 143]. This simple example shows that electromigration may be retarded due to the chemical potential gradient, created by precipitate coarsening. The electromigration flux of Al atoms can be simply represented as

$$J_{\text{Al}} = \frac{D_{\text{Al}} Z_{\text{Al}}^* \rho e}{kT} (j - \bar{j}_p) \quad (5.8)$$

where $\bar{j}_p$ represents the average critical current density imposed by the precipitate and is a function of precipitate spacing and the chemical potential gradient.

On the other hand, the migration rate of Cu is significantly enhanced. Once electromigration produces the coarsening situation, the migration rate is dominated by the diffusion force. At the grain boundary, the kinetics of Cu migration are expected to be faster both from the electromigration force and from the chemical potential force. It seems that this analysis contradicts Ho's estimate [19] of the lattice electromigration of Cu. Ho suggests that the migration of Cu is negligible in the Al lattice, because he found that the $Z_b^{**} \sim 0$ (see section 1.2). This result came from the fact that the estimated value of the vacancy flow effect (L_{ab}/L_{bb}) was -0.4, and the relative effective charge ratio, $Z_a^*/Z_b^* \sim 0.4$, so that $1 + (L_{ab}/L_{bb})(Z_a^*/Z_b^*) \sim 0$. However, the apparent effective charge of Cu, Z_b^{**} , cannot be zero or positive; Ho's result suggests that it is rather small. It should be noted that Ho's estimate was taken from the experimental value at the solid solution temperature. Even when the apparent effective charge of Cu in an Al lattice is small, a rapid migration of Cu is expected through the lattice if precipitates are present because once an electromigration force produces the coarsening situation described

above, the migration of Cu can be accelerated by the diffusion force. Cu migration was found to take place through the lattice, which qualitatively confirms the analysis. Of course, the migration of Cu was further enhanced by the injected vacancies from grain boundaries. Therefore, Ho's analysis is not necessarily contradicting the mechanism proposed here.

The net flux of Al and Cu atoms generates the vacancy flux. As proposed above, Cu migrates faster than Al atoms under the electromigration force: $J_{Cu} > J_{Al}$. In this case, the vacancy flux should move toward the dissolving precipitate and increase the vacancy concentration. The accumulated vacancies tend to form a void; this tendency can be counterbalanced by the enhanced diffusivity of vacancies at the dissolving precipitate. The diffusivity of Al atoms around a dissolving precipitate is significantly enhanced by the higher concentration of Cu, which means that the accumulated vacancies can out-diffuse to adjacent sinks such as the surface rather than exchanging sites with Cu in the precipitate. If the vacancy accumulation rate is comparable to the out-diffusion rate, the area around dissolving precipitates will be thinned during dissolution of a precipitate. After complete dissolution of the precipitate and reduction of the Cu to the solubility limit, voids can form easily because of the accumulation of vacancies and the reduced out-diffusion kinetics of vacancies. However, if the accumulation rate is faster than the out diffusion rate, voids will form at the precipitate site through the exchange of vacancies with Cu in the precipitate, while some vacancies out-diffuse to their sink.

In this mechanism, the problem is treated as interdiffusion of Al and Cu; the accumulation and depletion of Al atoms are not allowed in this treatment. However, in the real situation, the Al atoms will accumulate at the growing precipitate because it generates Al continuously. Therefore, the mass is accumulated at a growing precipitate, which can induce a compressive stress [141]. If a stress gradient is induced, the migration rate of Al atoms would be further reduced. As shown in the previous chapter, the study of the failure kinetics revealed that there exist significant healing mechanisms exist in fully

aged, wide lines, which resulted in the occasional decrease in the resistance after the damage formation. Unfortunately, the relative importance of the induced stress effect can not be proven.

5.5.3 Relation to the previous observations

Although the mechanism introduced in the above section is rather qualitative and simple, it provides an explanation for previous observations made by others [19-22, 39, 40, 142, 143], as well as observations made in this study. As summarized in the introduction, it was found that the Cu preferentially migrates. Also, void formation was generally observed after the complete depletion of precipitates, and when the concentration of Cu was reduced to approximately the solubility limit. All of these observations agree with the proposed mechanism. Now the simple postulation that precipitates act as a diffusion barrier for Al migration and as a vacancy sink can be justified. Precipitates act as effective diffusion barriers to Al migration because the coarsening driving force competes with the electromigration force. Precipitates act as vacancy sinks because they help the out-diffusion of vacancies at dissolving precipitates where vacancies accumulate. When the current density is small, or the microstructure allows a slow rate of vacancy accumulation, vacancies can be out-diffused without forming a void. If the vacancy accumulation rate is significant, either from a high current density or for microstructural reasons, some of the vacancies will exchange with Cu, forming a void at the precipitate. The current density used in this study was on the order of 10^6 A/cm^2 , which presumably induces a fast accumulation of vacancies in wide lines, and, therefore, a partial void was observed at the precipitate site.

Since the electromigration rate of Al atoms is effectively reduced by the presence of precipitates, and the formation of voids is retarded through out-diffusion, the electromigration lifetime of Al-Cu alloys can be significantly higher than for pure Al. It appears

that the ideal situation for the best performance against electromigration failure is to induce more stable precipitates with closer spacing. It takes a longer time to dissolve precipitates at the flux divergence sites, while the electromigration of Al atoms is effectively retarded, thus increasing the electromigration lifetime. This condition can not be achieved, however, in a real situation. When the alloys are aged to induce a more stable precipitate, the spacing between precipitates inevitably increases because the amount of Cu is limited. Fortunately, the location of precipitates is generally fixed at the triple grain junctions, so that aging can effectively enhance the electromigration lifetime. Also, the shorter spacing between precipitates is not necessarily beneficial, since the migration rate of Cu at shorter precipitate spacing increases from a higher concentration gradient, resulting in a faster sweep of the precipitate. Therefore, aging increases the electromigration lifetime, presumably because aging promotes the stabilization of precipitates separated by an optimum distance; this is applicable to the grain boundary failure mechanism found in wide lines. Since aging induces a loss of Cu or further separation of the precipitate at the failure site (bamboo grain), it is expected that there exists an optimum aging time for the best performance against electromigration failure; this is the case for narrow lines. In an optimum aging condition, both the Al and the Cu electromigration rate is relatively slow, so that vacancy out-diffusion to the film surface dominates the damage formation, resulting in diffuse thinning failure.

5.6 The role of alloying elements

Since all of the known alloying elements in Al form precipitates, the relation of electromigration and precipitate coarsening can be applied to other alloying systems. Experimentally it has been shown that Mg and Mn [1, 2, 80, 81], and transition metals such as Ti, Cr, and Ni [80-85] increase the electromigration lifetime. The electromigration lifetime significantly increases in Al-Mg alloys, when the concentration of Mg is

higher than the solubility limit [80, 81]. The increase of lifetime by the addition of transition metals are generally more significant than the addition of Cu, while it is often observed that voids form at the precipitate sites. On the other hand, the addition of Si, Ag and Au has little influence on the electromigration lifetime, although they do form precipitates [24].

In the interaction of precipitates and the electromigration force, it appears that four factors are important. The first factor is the diffusivity of the solute atom. Although precipitates can retard the electromigration of Al atoms, the retardation is only effective while the precipitate is existing within an effective distance. If the diffusivity of the solute atom is much faster than Al diffusivity, the precipitate dissolves much more rapidly, and the vacancy accumulation rate is faster, hence a void can easily form. The electromigration lifetime can not be enhanced by such alloying elements. Au and Ag fall into this category; they diffuse as low as 30 times faster than Cu in Al the lattice [119, 144]. On the other hand, when the diffusivity of the solute atom is comparable to or lower than the Al diffusivity, the electromigration lifetime can be significantly increased, since the dissolution kinetics of the precipitate are slow. Cu, Mg and transition metals fall into this category. The diffusivity of transition metals is significantly lower than the Al diffusivity [119], so that the expected lifetime enhancement would be significant with the addition of those alloying element. However, there is a second factor to be considered. A solute which can enhance the diffusivity of Al atoms is more beneficial because it can prevent the formation of a void. Transition metals are generally less effective in enhancing the diffusivity of Al than Cu [119], which promotes the formation of a void at the precipitate, where linkage of the voids fails the line. This is observed in Al-Cr and Al-Ti interconnects [146]. Third, the solute must produce an Al-containing precipitate, i.e., an intermetallic compound. If the solute precipitates as almost pure element, there would be no interaction between the electromigration force and the chemical potential force. Si is this type of alloying element. In terms of interaction between precipitates and the electromi-

gration force, the precipitate with a higher interfacial energy will be better for retarding the electromigration of Al atoms. This is because a higher interfacial energy produces a higher concentration gradient at a given precipitate size. Fourth, solutes that have lower solubility than Al are better because they can form more precipitates at a given amount of alloying addition.

The best choice for an alloying element for increasing the electromigration lifetime will be the solute that satisfies the above four requirements. For real applications, it seems that the solubility is the most important factor to consider. Low solubility can help to minimize undesired effects from the alloying element, such as increasing the electrical resistivity and susceptibility to corrosion, without losing the beneficial effect on the electromigration. Since information on diffusivity is not available, especially for grain boundary diffusion, suggestions can not be made with conclusive evidence. In terms of the solubility limit, Sc [146], W, Pd[147] and Zr appear to be good candidates.

5.7 Summary

The interaction of electromigration and precipitates is investigated in this chapter. Through the results of current reversal experiments it is concluded that the precipitates interact with the electromigration force; they are dissolved and grown by electromigration of Cu irrespective of the initial stability of the precipitate. It was also found that the sweeping rate of precipitates in polygranular segments influences the electromigration lifetime of narrow lines, although the effect was found to be smaller than that found after aging. This finding was deduced from the variation in the net mean time to failure and failure statistics. The result provides an explanation of why the bimodal distribution of failure statistics occurs in aged, narrow lines; the sweeping rate of precipitates at longer segments is slower, and the lifetime is longer than the expected lifetime which is extrapolated from the shorter segment length.

The interaction between precipitates and the electromigration force was phe

nomenologically expressed in the course of precipitate coarsening. It was qualitatively shown that Al electromigration can be retarded during precipitate coarsening, while the preferential migration of Cu is expected. As a result, the precipitate acts as a diffusion barrier to Al electromigration and as a vacancy sink. The proposed mechanism explains previous observations made in a study of Al-Cu electromigration, as well as the variation of electromigration lifetime with pre-aging presented in this study. An attempt was also made to provide a feasible explanation for the effect of other alloying elements on the electromigration lifetime, which might help to develop a better alloying system.

CHAPTER 6

STATISTICAL MECHANISM OF ELECTROMIGRATION FAILURE

As introduced in section 1.5.2.2, the statistical approach for electromigration failure mechanism contains fundamental problems when it is applied to the linewidth dependence of MTF and DTF. In the statistical approaches of electromigration failure, it was assumed that the thin film structure contains a fixed number of failure units with the time to failure t , and that these failure units are scaled with the grain size. For the serial connection of failure units where the time is determined by the weakest unit (first order statistics: eq. (1.38)), the mean time to failure (MTF) and the deviation of time to failure (DTF) changes with the number of failure units in a line, which scales with the effective linewidth (W/G). However, the time to failure of the first line should be the same for any linewidth, which contradicts the physical explanation.

The short coming of statistical models stems from the assumption that the distribution of failure units and their lifetimes are fixed regardless of the effective linewidth; only the number of failure units in a line scales with the linewidth. Also, the nature of failure units are not clearly defined, so that the number of units are rather arbitrary. Since the reliability of interconnects is determined by the low percent failure, it is essential to obtain the correct description of failure statistics, which will help to extrapolate the test data to the reliability limit.

The observations of failure mechanism in narrow lines (Chapter 4) can lead to the answer for the problem of the statistical model. The established failure mechanism suggests that the failure statistics are determined by the length distribution of polygranular segments. Based on these findings, a modified description of failure statistics is intro-

duced in this chapter in conjunction with the conventional statistical model. Since the study introduced in this chapter is intended to provide a guidance for further development of the model, the mechanism is qualitatively discussed.

6.1 Distribution of weak links in narrow lines

6.1.1 Normal distribution of weak links

It was found that the length of polygranular segments in 1.3 and 2 μm lines, measured by void-precipitate spacing, are normally distributed. A normal distribution is not a common distribution in thin film structure. However, in a statistical sense, a normal distribution is more realistic than any other distributions for the polygranular segment length. For simplicity, assuming square grains with the size of $d_1, d_2, \dots, d_N$, the length of polygranular segment, l_n , is then the sum of the grains within the polygranular segments, as schematically illustrated in Fig. 6.1:

$$l_{(n)} = d_1 + d_2 + \dots + d_n \quad (6.1)$$

where n represents the minimum number of grains to construct the polygranular segment. According to the central limit theorem (see Appendix A), any sum of a random variables with any distribution asymptotically approaches to normal distribution; although grain size is log-normally distributed, a linear sum of grains would follow a normal distribution.

As linewidth decreases, the number of grains in the polygranular segment would certainly decrease, and, correspondingly, the length of polygranular segment decreases as observed: the observed mean length of damaged units in 1.3 μm lines was 5.2 μm , while it was 6.9 μm in 2 μm lines. Also, it is expected that the number of polygranular segments per line slowly decreases with linewidth. However, the observed number of polygranular segment did not significantly vary with the linewidth: 8/line in 1.3 μm and

7/line in 2 μm lines. The estimation of damaged units were based on the fact that the void-precipitate pair appears at the polygranular segment, and, thus, it was possible that the some of polygranular segments were not counted due to the absence of the void-precipitate pair. Even though the observed number of polygranular segments slightly deviates from the expectation, we can assume that the length distribution of the polygranular segments is statistically the same as what was observed, for simplicity.

Fig. 6.1 A schematic illustration of polygranular segment assuming square grains.

As linewidth decreases, the polygranular segments are likely to be coarsely distributed. The standard deviation of the length distribution found in 1.3 μm lines was 2.15 μm , while it was 2.43 μm in 2 μm lines. It appears that the standard deviation is smaller in 1.3 μm lines in absolute scale; however, the shape parameter of the distribution, $\gamma = \sigma / \mu$, is the true measure of the distribution difference. The estimated γ is 0.41 for 1.3 μm lines and 0.35 for 2 μm lines, which indicates that the length distribution is coarser in narrower lines.

6.1.2 The distribution of the weakest units

The weakest link was the longest polygranular segment among all of polygranular segments in a line, which means that the weakest units are described by the n^{th} order statistics of the underlying distribution. When the cumulative distribution of the polygranular segment length l is

$$F(l) = \int_0^l f(l)dl \quad (6.2)$$

where $f(l)$ is the underlying distribution function of segment length, then for maximum extreme distribution, the probability of segment length, $G(l)$ is given by

$$G(l) = [F(l)]^{N_s} \quad (6.3)$$

where N_s represents the number of polygranular segments in a line. Since the segment length is physically valid only in the positive domain, the distribution function $f(l)$ is the truncated normal distribution function as defined in eq. (A.23)

Assuming that the underlying length distribution of the polygranular segments is the same as what was observed, the variation of the mean length and standard deviation with N_s can be calculated using eq. (6.3); these variations are shown in Fig. 6.2. The presented parameters are normally fitted values. These figures show that the mean length rapidly increase with N_s , while standard deviation exponentially decreases. The mean and standard deviation of the actual data that was taken from the length distribution of the failed segments are noted in the figures: $N_s = 8$ for 1.3 μm lines and $N_s = 7$ for 2 μm lines. There appears to be a good agreement between simulated values and the actual data. This analysis statistically confirms the statement that the failure occurs at the longest polygranular segment.

The observed distribution of the failed segment length was rather well fit to a normal distribution, which is same as the underlying distribution. When the underlying distribution is normal distribution, the maximum extreme distribution should be different

Fig. 6.2 The mean and standard deviation of the polygranular segment length as a function of the number of segments; the observed length distribution of damaged sites in (A) 1.3 and (B) 2 μm lines were used as the underlying distribution, i.e., $N_s = 1$.

Fig. 6.3 A plot of segment length distribution for (A) $1.3 \mu\text{m}$, and (B) $2 \mu\text{m}$ lines with two different segment numbers.

from the underlying distribution; however, it depends on N_s . The calculated extreme distribution function when $N_s = 8$ and $N_s = 100$ for 1.3 μm lines, and $N_s = 7$ and $N_s = 100$ for 2 μm , are compared in Fig. 6.3. The dotted lines represent the normal distribution. As shown in these figures, the maximum extreme distribution function of the segment length is reasonably well fitted to a normal distribution, although it is right-skewed. The maximum extreme distribution of normal distribution approaches to the asymptotic distribution as N_s approaches infinity, which is conventionally called a type I extreme value distribution of the largest, and it is described in Appendix A.

6.2 Statistics of electromigration lifetime

It has been shown that there exists a unique relation between the polygranular segment length and the time to failure, and the relation was justified through a diffusional model. The time to failure of polygranular segment l is given by

$$t_f = t_o \exp\left(-\frac{l}{l_o}\right) \quad (6.4)$$

or

$$l = l_o [\ln t_o - \ln t_f] \quad (6.5)$$

where t_o and l_o are defined in eq. (4.8) and (4.9), and are a function of linewidth. Since the underlying distribution of the polygranular segment lengths is a normal distribution, the time to failure of the polygranular segments is a log-normal distribution, which follows the relation:

$$f(t_f) = \frac{1}{t_f \sigma_f \sqrt{2\pi}} \exp\left(-\left(\frac{\ln t_f - \ln t_{50}}{2\sigma_f}\right)^2\right) \quad (6.6)$$

where σ_f denotes the shape parameter of the log-normal distribution, or simply DTF. From eqs. (6.5)-(6.6), it can be shown that the DTF of narrow lines is determined by the

standard deviation of the length distribution (σ) and l_0 :

$$\sigma_f = \frac{\sigma}{l_0} = \frac{Z^* e \rho j}{kT} \sigma \quad (6.7)$$

This equation predicts that the DTF would be larger when the lines are tested at higher current density and lower temperature for a given line structure.

There have been various models [60, 61, 148], that predict the variation of DTF with the test temperature and current density. All of these models have adapted the same assumption that a certain physical property has a normal distribution. Babbio and Saracco [61] proposed that the actual test temperature of each line can vary due to variations in the thermal characteristics and testing conditions of the lines. If the variation in temperature come from a variation in the heat transfer rate, H , then from eq. (2.4), $1/T$ is given by

$$\frac{1}{T} = \frac{H}{\rho j^2} \quad (6.8)$$

If the variation in H has a normal distribution with a standard deviation of σ_H , then DTF is given by

$$DTF_H = \frac{E_a}{k \rho j^2} \sigma_H \quad (6.9)$$

On the other hand, Lloyd [60] assumed that T has a normal distribution, thus giving DTF,

$$DTF_T = \frac{E_a}{kT^2} \sigma_T \quad (6.10)$$

where σ_T is the standard deviation in the line temperature. Based on these assumptions a larger DTF would be expected when lines are tested at lower current densities, lower temperature and for higher activation energy materials. These predictions are slightly different from what was derived in eq. (6.7). However, the above models assume that the DTF dependence on T and j is from variations in the test conditions not from the physi-

cal difference in the failure mechanism. If narrow lines are tested with the various test conditions assumed by others, the resulted DTF would be the combination of those three contributions, and it would be given as

$$DTF = \sqrt{\sigma_f^2 + DTF_H^2 + DTF_T^2} \quad (6.11)$$

If tests are done under well controlled condition, the DTF dependence on current density would follow eq. (6.7).

Although the time to failure data has consistently been found to have a log-normal distribution [51-53], there have been some arguments for other distributions [52, 149-151]. Towner [52] found that the lifetime of Al interconnects fit well either a log-normal distribution or the Type III extreme value distribution of the smallest (Weibull distribution) when the linewidth is comparable to or smaller than the mean grain size. A type III distribution of the smallest is left-skewed to a log-normal distribution. Lloyd [150] proposed a multi-log-normal distribution for narrow lines. The argument for a log-normal distribution in narrow lines stems from the basic assumption of the statistical model. According to the statistical model, the time to failure of failure units has a log-normal distribution. Since the failure occurs at the weakest units, the apparent distribution should have a smallest extreme value distribution (Weibull). However, the experimentally observed distribution is usually a log-normal not a Weibull, which causes a dilemma in statistical model. A log-normal distribution is not self-reproducible, which means that the extreme value distribution of a log-normal distribution can not be a log-normal distribution.

The observation made in this study may provide a way to overcome the dilemma of the failure statistics. As discussed above, the origin of a log-normal distribution is generated by the normal distribution of the polygranular segment length and their logarithmic dependence on the failure time. If the number of polygranular segments, N_s , in a line is relatively small, the polygranular segment length can still be well fitted by a nor-

mal distribution (Fig. 6.3), and, thus, the lifetime can be fitted log-normally. When the number of segment is infinitely large, the distribution of lifetime asymptotically approaches to the Weibull distribution. In other words, the type of apparent distribution is a function of unit numbers. The number of units vary with the linewidth and length. This argument should be examined as a function of those physical parameters of interconnects as included in the following discussions. It will be shown that the Weibull distribution is difficult to obtain in any case.

6.3. Linewidth dependence of failure statistics

As already pointed out in the section 4.4.4, the MTF and DTF of narrow lines depends on the linewidth because of the variations in the failure kinetic parameters t_o , l_o and polygranular segment length l in eq. (6.4).

As the linewidth decreases in narrow lines, the length of polygranular segments decreases, and, thus, the corresponding lifetime increases with the accompanying variation of t_o and l_o . From eq. (6.5), it can be proposed that MTF qualitatively varies with the linewidth as

$$MTF = t_o(w) \exp\left(-\frac{l_m(w)}{l_o(w)}\right) \quad (6.12)$$

where w and l_m denote the effective linewidth (W/G) and the mean length of the polygranular segments, respectively. As the linewidth decreases in narrow lines it was found that t_o and l_o increases, while l_m decreases. Therefore, it can be qualitatively assumed that $t_o(w)$ is inversely proportional to w , and $l_m(w)$ and $l_o(w)$ are linear functions of linewidth as a first principle approximation. The relation of each parameter to w , referenced to the parameters at critical width $w = 1$, can be given as

$$\begin{aligned} t_o(w) &= A t_o(1) / w \\ l_m(w) &= B l_m(1) w \end{aligned} \quad (6.13)$$

$$l_o(w) = Cl_o(1)w$$

where A, B and C are the correlation constants, and then

$$MTF = \frac{At_o(1)}{w} \exp\left(-B' \frac{l_m(1)}{l_o(1)}\right) \quad (6.14)$$

Eq. (6.14) indicates that MTF rapidly increases as w decreases.

DTF depends on the distribution of the polygranular segment. As demonstrated previously, the shape parameter γ of the length distribution decreases with the effective linewidth: when $w = 0.83$ (2 μm lines), $\gamma = 0.35$, and when $w = 0.54$ (1.3 μm lines), $\gamma = 0.41$. If we assume that γ is inversely proportional to w , then from eq. (6.7), it becomes

$$DTF = C' \frac{\sigma(1) l_m(1)}{w l_o(1)} \quad (6.15)$$

where C' is the correlation constant. Eq. (6.15) also indicates that DTF should rapidly increase as w decreases. Eqs. (6.14) and (6.15) provide qualitatively correct descriptions of MTF and DTF dependence on the linewidth, which was not completely answered in either the physical or statistical models.

As linewidth decreases, the number of polygranular segments is expected to decrease. Therefore, the lifetime data should be best fitted to a log-normal distribution.

6.4 Line length dependence of failure statistics

In a given linewidth the number of polygranular segments increases with increasing line length. In this case, the mean and the standard deviation of polygranular segment length decrease rapidly as shown in Fig. 6.2. Accordingly, the MTF and DTF are expected to decrease. In order to demonstrate the line length effect on MTF and DTF the experimentally determined l_o and t_o (Fig. 4.25) were taken and applied to the simulated statistics of polygranular segments shown in Fig. 6.2. The results are shown in Fig. 6.4 as

Fig. 6.4 MTF and DTF for (A) 1.3 and (B) 2 μm lines as a function of the number of polygranular segments in a line. The corresponding line length is also noted in the figure.

a function of the segment number, N_s . Experimentally determined MTF and DTF are noted in the figures ($N_s = 8$ and $N_s = 7$). Since the test line length was $800 \mu\text{m}$, the average spacing between each segment is about $100 \mu\text{m}$; based on this estimation, the equivalent line length was also noted. It can be seen that the MTF and DTF exponentially decrease with the line length in both linewidths and approach a minimum value for large N_s . In this calculation, only the number of failure units are varied using a given underlying distribution. Hence, this is the same method as the conventional model for the simulation of linewidth effect on MTF and DTF. This analysis indicates that the conventional statistical model is an adequate choice for the line length effect but not for the linewidth effect.

The line length dependence of MTF and DTF also varies with the linewidth in the sense that the linewidth changes the underlying distribution of polygranular segment length, the number of segments per a given length, and the failure kinetic factors t_0 and l_0 . Qualitative equations for the line length dependence of MTF and DTF on the linewidth can be constructed as in eqs. (6.14)-(6.15), assuming that the number of failure units or the polygranular segment per unit length scales with linewidth. Let L be a length of the test line, and then the number of units at critical linewidth can be approximated as $N_s(1) \sim Kl_m(1)/L$, where K is a constant. The number of units at arbitrary width, $N_s(w)$, decreases with linewidth, and, thus, we can assume that the relation is linear:

$$N_s(w) = K' \frac{l_m(1)}{L} w \quad (6.16)$$

where K' is a constant. An analysis revealed that the MTF and DTF is an exponential function of N_s , i.e., $\sim \exp(-N_s)$, so that the MTF and DTF can be approximated as

$$\begin{aligned} MTF &\approx \frac{At_o(1)}{w} \exp\left(-B' \frac{l_m(1)}{l_o(1)} - K' \frac{l_m(1)w}{L}\right) \\ DTF &\approx C \frac{\sigma(1)}{w} \frac{l_m(1)}{l_o(1)} \exp\left(-K' \frac{l_m(1)w}{L}\right) \end{aligned} \quad (6.17)$$

It can be seen that MTF and DTF decrease rapidly with increasing line length L , and the relative variation is influenced by the effective linewidth, w ; the variations of MTF and DTF is smaller and slower when w is narrower. The magnitude of MTF and DTF variation in this line is greater than wider lines; this can be seen from the comparison of the simulated results of 1.3 μm and 2 μm lines shown in Fig. 6.4. However, the saturation of MTF and DTF appears more quickly in wider lines because the number of polygranular segment per a given length is much smaller. In other words, to increase the same number of units, narrower line needs longer increment of line length. This does not appear in Fig. 6.4 because the number of polygranular segments are close to each other; however, it can be seen that, in both cases, the saturation of MTF and DTF appears when the line length is about 1 cm. Eq. (6.17) provides qualitative insight for the linewidth and length dependence of MTF and DTF of electromigration failure.

According to experiments by Agarwala *et al.*, performed on wide Al lines, the MTF and DTF decreases rapidly and saturated at the line length of 125 to 500 μm [73]. Learn *et al* [152] found that the length dependence of MTF and DTF is a function of grain size. For a large-grained film, as the line length was increased from 125 to 1250 μm and 1250 to 5000 μm , MTF decreased by a factor 10.6 and 1.5, respectively. However, for a small-grained film, MTF only decreased by a factor of 4.3 and 1.3, respectively. Tests on large-grained material is equivalent to tests at narrower linewidth. Schafft *et al* [56] found that for 3.0 μm -wide Al-1%Si lines, the MTF decreased 16% and 5% when the line length was increased from 400 μm to 800 μm and from 800 to 1200 μm , respectively. These observations fit the qualitative model developed above if the effective linewidth is adapted. For wide lines, the MTF and DTF quickly saturate with little variation, while, in narrow lines, the saturation is slower but the variation of the magnitude is higher. If the linewidth is narrow enough, such that the line can contain very few polygranular segment in a very long line length, the change of MTF and DTF can not be easily detected unless the line is long (for example, saturation will appear when the length of the lines tested is

this study is greater than 1 cm). Kwok [76] reported nearly identical MTF and DTF for submicron lines, independent of line length, which appears to be the case.

The distribution of lifetimes will be changed by the line length, from a log-normal to Weibull, because N_s increases as line length increases. However, a log-normal distribution would fit the lifetime distribution reasonably well unless narrow lines of extremely long length are tested. Although the lines with linewidth around the critical width can provide a large number of failure units in a moderate line length, the weaker dependence of time to failure on segment length, and, thus, increasing influence from each grain boundary in the segment to the time to failure, will make the lifetime fit to log-normal distribution. In short, a log-normal distribution is a good measure for the lifetime statistics. It should be also noted that a log-normal distribution is very flexible distribution. The argument of log-normal distribution introduced so far ignores the influence of precipitates. As proved in this study, when the time to failure of polygranular segment is strongly influenced by the secondary microstructural factors such as precipitation, it appears that a multi-log-normal distribution would be the right choice; the development of multi-log-normal distribution by microstructural factors should be explored.

6.5 Summary

Using the observations presented in chapter 4, the statistical aspects of electromigration failure in narrow lines are studied. The statement that the failure occurs at the longest polygranular segment is examined using n^{th} order statistics, and the results confirm the statistical nature of failure in narrow lines.

In narrow lines the polygranular segments act as failure units, and the longest segments are the weakest units. The scaling of the units is not independent of linewidth, as assumed in the conventional models; as the linewidth decreases, the number and the length of the polygranular segments decreases with coarser distribution. As the segment

length decreases MTF increases, while coarser distribution increases DTF. Hence, the MTF and DTF dependence on linewidth comes from a physical difference of the lines, not only from the statistical nature of unit scaling, which provides the answer for the gap between the previous models.

The number of polygranular segments also scales with line length. The longer line can contain more polygranular segments, and, thus, the probability to have a longer segment increases, while the distribution becomes more uniform. As a result, the MTF and DTF also depend on the line length; they rapidly decrease to saturation values as the line length increases. Since the scaling of the number of polygranular segments depends not only on line length but also on linewidth for a given microstructure, there exists a linewidth dependence of MTF and DTF; it was found that MTF and DTF saturate more rapidly with smaller variation in wider lines.

CHAPTER 7

CONCLUSIONS AND FUTURE WORK

7.1 Conclusions

The mechanism of electromigration failure in Al thin films is strongly influenced by the microstructural parameters of the thin films, such as grain size and precipitate distribution. In this study, the influence of these parameters is investigated by varying the effective linewidth for a fixed microstructure, and pre-aging of lines to induce various distribution of precipitates.

For wide lines ($W/G > 1$), the failure mechanism is governed by grain boundary electromigration. Voids nucleate and grow to failure along the grain boundary. However, for narrow lines ($W/G < 1$) which have predominantly a bamboo grain structure with occasional polygranular segments, failure occurs at the bamboo grain that terminates a polygranular segment, producing a slit-like void. Transgranular failure occurs through accumulation of vacancies after Cu has been swept from the grain that fails. The time to failure, determined by the longest polygranular segment in the line; it exponentially decreases with linear increase of the segment length. The decrease is more rapid in narrower lines, while the pre-exponential constant is higher in narrower lines.

Since the length of a polygranular segment determines the time to failure, the statistics of polygranular segment length fixes the failure statistics. The statistical distribution of polygranular segments is determined by the film microstructure and is a function of effective linewidth; as effective linewidth decreases, the mean polygranular length decreases, while the fractional deviation increases, so that MTF and DTF increase, ac-

cordingly. At a given linewidth, the number of polygranular segments scales with line length, and, therefore, MTF and DTF also depends on the line length.

Pre-aging lines causes Cu to precipitate at the interior of grains and grain boundaries. Since the grain size in thin films is small enough to put intragranular precipitates in the diffusion field of the grain boundary, the type and distribution of intragranular precipitates evolves with the aging time, while grain boundary precipitates continuously grow. For wide lines, precipitates at grain boundaries retard the electromigration failure, and, thus, the lifetime linearly increases with pre-aging time. On the other hand, failure in narrow lines requires precipitates to be swept from grains that fail, causing lifetime to evolve with aging time; a more stable and dense distribution of intragranular precipitates lengthens the time required to sweep precipitates within a bamboo grain, which substantially increase the lifetime. In the optimal case, the transgranular failure mechanism is suppressed and the line fails by diffuse thinning. The time to sweep precipitates in a polygranular segment, although it is relatively short compared to the time to sweep Cu in bamboo grains, preferentially increases the time to failure of a longer segment, and, as a result, a bimodal distribution of lifetime is developed with pre-aging.

Precipitates retard the electromigration failure because they act as a diffusion barrier for electromigration of Al atoms and as an effective vacancy sink. Precipitates are dissolved and coarsened by the electromigration force, which induces a chemical potential gradient. This induced chemical potential gradient pushes Al atoms to the opposite direction of the electromigration force, while it accelerates the migration of Cu atoms in the direction of electromigration force. Hence, electromigration of Al atoms is retarded by the presence of precipitates, while migration of Cu atoms is enhanced. In addition to this, the accumulated vacancies at the dissolving precipitate, which is generated by the net Cu and Al flux, can be annihilated through out-diffusion to the film surface because of enhanced diffusivity by high concentration of Cu around it; this also retards the electromigration failure. Therefore, pre-aging of lines to create stable precipitates which can

retard electromigration while they dissolve is an effective method to enhance the reliability of interconnects.

7.2 Future work

7.2.1 Current exponent and failure statistics in narrow interconnects

The time to failure of the polygranular segment is an exponential function of its length, following the relation defined in eq. (4.7). If eq. (4.7) is represented as a function of current density, j , it becomes

$$t_f = t_o \exp\left(-\frac{j}{j_o}\right) \quad (7.1)$$

where j_o is the effective current density under which no electromigration occurs. Hence, the MTF varies exponentially with current density, following the relation

$$MTF = A' \exp\left(-\frac{j}{j_o}\right), \quad (7.2)$$

which is different from the conventional expression (Black's equation):

$$MTF = Aj^{-n} \quad (7.3)$$

where A and A' are the correlation constants. An experiment measuring MTF for various current densities, keeping linewidth and microstructure constant, would confirm that eq. (7.2) is the correct relationship between MTF and current density for narrow lines.

If stress driven back diffusion has a significant influence on the failure rate, from eq. (4.13), eq. (7.2) should be modified as

$$MTF = A \exp\left(-\frac{j}{j_o} + S\right) \quad (7.4)$$

where S represents the contribution of the stress driven back diffusion on the failure time:

$$S = \frac{\Omega \Delta \sigma}{kT} \quad (7.5)$$

It can be seen that the stress factor S is not a function of current density, rather it simply increases the MTF by the same amount for all current densities.

The above analysis can be confirmed by a study of the current exponent performed as a function of effective linewidths. As the effective linewidth of narrow lines decreases, the critical current density j_0 increases. Therefore, the MTF varies more rapidly with current density in narrower lines. However, the absolute scale of MTF increases in narrower lines because the stress factor S simply increases the MTF to the higher values: the induced stress will be higher in narrower lines for a given amount of mass accumulation. Such a study would reveal the relative importance of stress driven back diffusion and diffusional back flux.

7.2.2 Reliability improvement of narrow interconnects

This study showed that the reliability can be actually increased by reducing the effective linewidth of interconnects. However, it should be noted that reducing linewidth is a limited solution because the benefit is counterbalanced by an increase in the current density. Post heat treatment to increase the grain size would be advisable, making effective linewidth smaller without increasing current density. The optimal heat treatment would produce large grains of uniform size.

The aging of alloyed interconnects is also an effective way to enhance the reliability. Although the general idea is introduced in this study, an intensive investigation is necessary to obtain the best aging conditions. It should be noted that aging is not necessarily beneficial for every case. When the grain size of the films is relatively small, it is not possible to obtain the maximum density of stable precipitates in grains, as discussed in chapter 3. Additionally, formation of blocky precipitates in bamboo grain boundary would be detrimental because they causes local heating around them due to their high re-

sistivity. Therefore, a combination of heat treatments which optimize the grain structure and precipitate distribution would be ideal.

7.2.3. Precipitation under electromigration

Electromigration force introduces a directionality of Cu migration, resulting in inhomogeneous precipitation of Cu, as shown in this investigation. Phenomenologically, it is expected that the precipitation rate in Al-Cu alloys is enhanced by electromigration force due to enhanced diffusivity of Cu; however, this has not been experimentally explored yet because of the complexity involved in the experiment and the analysis.

Electromigration increases the vacancy concentration in the lattice. There are several possible influences from the increased vacancy concentration on the precipitation of Cu. The enhanced diffusivity of Cu may simply accelerate the sequence of precipitation. If vacancies form small clusters, they can provide nucleation sites for stable precipitates. Therefore, the direct nucleation of θ precipitates without GP zone stages might be possible. These precipitates should be small in their size due to the limited size of vacancy clusters. Although it is not solidly confirmed, finely dispersed and extremely small θ precipitates were found in the samples that were exposed to the electromigration. The size of these precipitates were on the order of a few hundreds of nano-meters, which is much smaller than that of θ' .

Study of precipitation under high current density is usually complicated due to the complex microstructure of thin films. It would be advantageous to grow an Al-Cu single crystal, so that precipitation characteristics can be investigated without influence from grain boundaries. The interaction of precipitates and electromigration can also be studied by making a bi-crystal in which a grain boundary is artificially fabricated. When this single grain boundary is fabricated to have a specific angle to the line direction, the dissolution and growth of θ precipitates, and the relative kinetics of Al and Cu electromigration can be quantified.

APPENDIX A

STATISTICS FOR ELECTROMIGRATION

The study of electromigration failure in thin films of Al and Al alloys requires statistical analysis due to the statistical process of electromigration failure. Although there are many important theories on the statistics of electromigration [153-158], the understanding of the basic properties of statistical distributions is the most crucial. For this reason, basic concepts and properties of various distributions including the normal and log-normal distributions are briefly introduced in this section.

A.1 Basic concepts

A.1.1 Probability density function

Consider the probability of the continuous random variable X taking a measurement value in the interval $(x-dx/2, x+dx/2)$. As a function of x , this probability value can be considered in terms of *probability density function*, or simply *density function*, $f(x)$ as

$$\Pr(x - \frac{dx}{2} \leq X \leq x + \frac{dx}{2}) = f(x)dx \quad (A.1)$$

The density function is abbreviated as "p.d.f."

A.1.2 Cumulative distribution function

Instead of studying the probability density function of measurement values x , it is often instructive to consider the probability of obtaining any measurement below a value x . Thus the probability function of interest is now $\Pr(X < x)$. This function is called a *cumulative distribution function*, denoted as $F(x)$, abbreviated as c.d.f., and defined as

$$F(x) = \Pr(X \leq x) \quad (\text{A.2})$$

Now, $F(x)$ can be expressed in terms of $f(x)$, for a continuous random variable X , as

$$F(x) = \int_{-\infty}^x f(x) dx \quad (\text{A.3})$$

Similarly, $f(x)$ can be derived from $F(x)$ as

$$f(x) = \frac{d}{dx} F(x) \quad (\text{A.4})$$

A.1.3 Moments

One of the most important concepts in statistical work is that of a mathematical expectation (or expected value). Let $g(X)$ be a function of a continuous random variable X , and let $f(x)$ be the p.d.f. of X . The mathematical expectation of $g(X)$ is then represented as

$$E\{g(X)\} = \int_x g(x) f(x) dx \quad (\text{A.5})$$

provided that the integral converges absolutely. Some useful expectations follow from eq. (A.5). If k is constant, we have

$$\begin{aligned} E\{k\} &= k \\ E\{(kg(x))^r\} &= k^r E\{g^r(x)\} \\ E\{k_1 g_1(x) + k_2 g_2(x)\} &= k_1 E\{g_1(x)\} + k_2 E\{g_2(x)\} \end{aligned} \quad (\text{A.6})$$

Consider the special case $g(X) = X$. Eq. (A.5) then becomes

$$E\{X\} = \int_x x f(x) dx \quad (\text{A.7})$$

and is called the *expected value of X* , or simply the *mean of X* . It is seen to be the weighted average of the random variable X with respect to its p.d.f. $f(x)$. More generally, let the function $g(X)$ take the special form $g(X) = (X-A)^r$, where A and r are constants. Then we have

$$E\{(X - A)^r\} = \int_x (x - A)^r f(x) dx \quad (\text{A.8})$$

which is called r^{th} moment of X about the point A , in analogy with the moments of mechanics. The constant A is a point on the measurement axis of x and therefore has the same dimension as x . If the constant A is taken as the mean value of X , then the resulting expectation is termed the r^{th} central moments of X or the r^{th} moment of X about its mean. This moment is often denoted as $m(r)$, where

$$m(r) = E\{(X - E\{X\})^r\} \quad (\text{A.9})$$

If, on the other hand, the constant A is taken to be the origin of the measurement axis of x , $A = 0$, the expectation (A.9) is termed the r^{th} moment of X . This moment is denoted as

$$m(r)' = E\{(X)^r\} \quad (\text{A.10})$$

The most frequently used moments are those for $r = 1$ and $r = 2$. From eq. (A.6) and (A.9), it is seen that for $r = 1$, $m(1) = 0$. For $r = 1$, eq. (A.10) reduces to the mean value of X , $m(1)' = E\{X\} = \mu$. For $r = 2$, eq. (A.9) gives the *second central moment* of X , termed the *variance* of X :

$$m(2) = \sigma^2 = E\{(X - E\{X\})^2\} \quad (\text{A.11})$$

where σ denotes the standard deviation. The moments $m(1)'$ and $m(2)$, or the mean μ and variance σ^2 , describe aspects of the appearance of the distribution $f(x)$. The mean μ is a measure of location indicating where the *bulk* of the probability is located on the measurement axis of x . Similarly, the standard deviation of X , σ , is a measure of dispersion, indicating the *spread* exhibited by the model $f(x)$.

Since $m(1)' = E\{X\}$ is a constant, the variance of X , $m(2)$ can be expressed as

$$\begin{aligned} m(2) &= E\{(X - m(1)')^2\} = E\{X^2 - 2xm(1)' + (m(1)')^2\} \\ &= E\{X^2\} - (E\{X\})^2 \end{aligned}$$

$$= m(2)' - [m(1)']^2 \quad (\text{A.12})$$

In this form the variance $m(2)$ can often be computed quite easily. Similarly, it can be shown that

$$m(3) = m(3)' - 3m(1)' m(2)' + 2[m(1)']^3 \quad (\text{A.13})$$

$$m(4) = m(4)' - 4m(1)' m(3)' + 6[m(1)']^2 m(2)' - 3[m(1)']^4 \quad (\text{A.14})$$

A.1.4 Order statistics

Consider the largest sample value X_n among n independent (unordered) sample values X_i with the p.d.f. $f(x_i)$. If this random variable X_n takes on a value that is less than or equal to x , it follows that all other realizations x_i must likewise be less than or equal to x . Hence the statement $X_n < x$ is equivalent to the statement $X_i < x$, for all i . Thus, if a number of samples of size n is taken, the cumulative relative frequency of occurrence of $X_i < x$ is precisely equal to the cumulative relative frequency of occurrence of $x_i < x$, for all i . Since the proceeding relative frequency is the product of n identical relative frequencies of the measurement event $X_i < x$, the c.d.f. G_n of the random variable X_n is given by the product $[F(x)]^n$. That is,

$$G_n(x; n) = [F(x)]^n \quad (\text{A.15})$$

and the p.d.f. of the n^{th} order statistics X_n is obtained as

$$g_n(x; n) = \frac{d}{dx} G_n(x; n) = n[F(x)]^{n-1} f(x) \quad (\text{A.16})$$

Similarly, if the smallest sample value X_1 is larger than a given value x , it follows that all sample values X_i must be larger than x . Thus cumulative relative frequency of occurrence of $X_1 > x$ equals the cumulative relative frequency of occurrence of $X_i > x$, all i . That is,

$$[1 - G_1(x; n)] = [1 - F(x)]^n \quad (\text{A.17})$$

so that the c.d.f. of the first order statistics X_1 is obtained as

$$G_1(x;n) = 1 - [1 - F(x)]^n \quad (\text{A.18})$$

The equivalent p.d.f. of X_1 is

$$g_1(x;n) = n[1 - F(x)]^{n-1} f(x) \quad (\text{A.19})$$

In general, for r^{th} order statistics X_r (the r th-smallest samples value), the p.d.f. $g_r(x;n)$ has the form as

$$g_r(x;n) = \frac{n!}{(r-1)!(n-r)!} [F(x)]^{r-1} [1 - F(x)]^{n-r} f(x) \quad (\text{A.20})$$

The n^{th} and the first order statistics derived here are particularly useful in many engineering applications such as lifetime statistics, since n th order statistics represents the maximum choice of a variable among others, while the first order statistics represent the minimum choice of physical variables which often determine the lifetime of sample.

A.2 Normal distribution

A.2.1 Definition

A random variable X is normally distributed with mean μ ($-\infty < \mu < \infty$) and variance σ^2 ($\sigma > 0$) if the probability density function of X is given by

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} \quad (\text{A.21})$$

where $-\infty < x < \infty$. The parameter μ is both the mean and median, and σ is the standard deviation of the normal distribution. If the random variable X is defined only in the positive domain, as in case of lifetime, the truncated normal density function should be used as

$$f(x) = \frac{1}{k\sqrt{2\pi}\sigma} \exp\left[-\left(\frac{x-\mu}{\sqrt{2}\sigma}\right)^2\right] \quad (\text{A.22})$$

where k is referred to as the normalizing constant and is such that

$$\int_0^{\infty} f(x) dx = 1 \quad (\text{A.23})$$

The moments of the normal distribution defined as

$$m(r)' = \int_{-\infty}^{\infty} x^r f(x) dx \quad (\text{A.24})$$

are

$$\begin{aligned} m(1)' &= \mu \\ m(2)' &= \mu^2 + \sigma^2 = \mu^2 (1 + \gamma^2) \\ m(3)' &= \mu^3 + 3\mu\sigma^2 = \mu^3 (1 + 3\gamma^2) \\ m(4)' &= \mu^4 + 6\mu^2\sigma^2 + 3\sigma^4 = \mu^4 (1 + 6\gamma^2 + 3\gamma^4) \end{aligned} \quad (\text{A.25})$$

where $\gamma = \sigma / \mu$, called shape parameter of the normal distribution. The shape parameter γ is dimensionless, and, thus, it allows the comparison of several distributions with different mean and standard deviation. The normal density distribution function can be standardized by linearly transforming the random variable X as $Z = (x - \mu) / \sigma$. Thus, the cumulative distribution function of a standard normal random variable is defined as

$$\Phi(Z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^z \exp(-\frac{u^2}{2}) du \quad (\text{A.26})$$

The actual cumulative distribution function, $F(x)$, of any normal random variable with mean μ and variance σ^2 can then be expressed in terms of Φ ;

$$F(x) = \Phi\left(\frac{x - \mu}{\sigma}\right) \quad (\text{A.27})$$

A.2.2 Central limit theorem

Let $X_1, X_2, \dots, X_n$ be an independent identically distributed random variables with a distribution that features an expected value μ and a finite variance $\sigma \neq 0$. The average value statistics

$$Y = \bar{X} = (1/n) \sum_{i=1}^n X_i \quad (\text{A.28})$$

then has a limiting distribution which is normal, with expected value $m(1)' = \mu$ and variance $\sigma^2 = m(2)/n$. This theorem means that as the chosen sample size n increases, the sta-

tistical model of the sample average Y tends to the normal model with expected value $m(1)'$ and standard deviation $\sqrt{m(2)/n}$.

An even more powerful limit theorem states that the sampling model of the statistics $Y = \bar{X}$ tend to normality even if the individual sample X_i have different distribution, provided that each random variable X_i has a finite third moment $m(3)'$. In this case, the average value statistics $Y = \bar{X}$ has a limiting distribution which is normal with expected value

$$\mu = \frac{1}{n} \sum_{i=1}^n m(1; X_i) \quad (\text{A.29})$$

and variance

$$\sigma^2 = \frac{1}{n^2} \sum_{i=1}^n m(2; X_i) \quad (\text{A.30})$$

This is known as the central limit theorem. In other words, any sum of random variables with any distribution has the normal distribution. The required number of variables n to produce well behaving normal distribution depends on the distribution of variable X .

A.2.3 Probability paper

Probability paper provides a qualitative but simply way to fit data to a certain distribution and determine the distribution parameters. Normal probability paper is designed so that normally distributed random variables lie on a straight line. From eq. (A.28), the value of random variable X can be written as

$$X = \mu + \sigma \Phi^{-1}(F) \quad (\text{A.31})$$

where Φ^{-1} is the inverse function of the standard normal cumulative distribution function. If X is plotted against $\Phi^{-1}(F)$, it will have a linear relationship with slope σ and intercept μ . The construction normal of probability paper is illustrated in Fig. A.1. The

Fig. A.1 Construction of normal probability paper; (A) probability density function of the standard normal distribution, and (B) normal probability paper: the y-axis is the linear data scale and the x-axis is the probability scale that has the value F located at $\Phi^{-1}(F)$.

cumulative probability F is defined as $n / (N+1)$, where N is the total number of data, and n is the number of data in the probability. In order to plot the last probability, i.e. 100 % probability, $N+1$ is used in the denominator instead of N .

The mean and standard deviation can be obtained by least squares method on normal probability paper. The intercept at 50 % probability corresponds to the mean μ . The slope of the fitted line represents the standard deviation and can be approximated as

$$\sigma \sim \mu - X_{16\%} = \mu - X_{84\%} \quad (\text{A.32})$$

since $\Phi^{-1}(0.16) = -1$, and $\Phi^{-1}(0.84) = 1$

A.3 Log-normal distribution

The log-normal distribution is very flexible distribution, because it has a great variety of shapes. Because of its versatility, it is used in many engineering statistics such as for light emitting diodes [159, 160], electromigration failure of interconnects, fatigue lifetime of metals [161, 162] and grain size distribution of thin films.

A.3.1 Definition

When a random variable X is normally distributed with mean μ and variance σ^2 , the new variable $\{t\}=e^X$ is log-normally distributed. In other words, $\ln t$ is normally distributed with mean μ and variance σ^2 . Due to the similarity of the log-normal distribution to normal distribution, the analysis for the normal distribution can be used for the log-normal distribution. Transforming a log-normal random variable T to a standard normal variable Z , i.e., $Z = (\ln t - \mu)/\sigma$, the cumulative distribution function of log-normal distribution, $F(t)$, can be obtained as

$$F(t) = \Phi\left(\frac{\ln t - \mu}{\sigma}\right) \quad (\text{A.33})$$

where Φ is the distribution function of the standard normal distribution. The density function of the log-normal distribution is then given by

$$f(t) = \frac{dF}{dt} = \frac{1}{t\sqrt{2\pi}\sigma} \exp\left[-\left(\frac{\ln t - \mu}{\sqrt{2}\sigma}\right)^2\right] \quad (\text{A.34})$$

Here, the variable t is only defined in the positive domain. The shape of the log-normal distribution is monomodal and positively skewed. The mean of the log-normal distribution is $\exp(\mu)$ is often called t_{50} . The standard deviation of log-normal distribution is dimensionless because it is the deviation of $\ln t$, not of t , and, thus, it is often called shape parameter of the distribution. Although a log-normal distribution is similar to a normal distribution, the meaning of μ and σ are different from that of a normal distribution. Clearly, the parameters μ and σ are not location or scale parameter, rather σ is a shape parameter and $\exp(\mu)$ is a scale parameter of the distribution function. The moments of a log-normal distribution can be obtained from the moments generation function defined in eq. (A.25), and they are

$$m(r) = \exp(r\mu + \frac{r^2\sigma^2}{2}) = t_{50}^r \exp(\frac{r^2\sigma^2}{2}) \quad (\text{A.35})$$

A.3.2 Origin of the log-normal distribution

Normal distribution results from the additive effects of a combination of randomly distributed variables, as seen from the central limit theorem. Similarly, log-normal distribution comes from the multiplicative effects of variables or combination of such variables. If a random variable Y is the product of n independent positive random variables,

$$Y = \prod_{i=1}^n T_i \quad (\text{A.36})$$

then Y is asymptotically log-normally distributed. An example of log-normal distribution can be seen from the analysis of lifetimes of metal fatigue, which is known to be log-normally distributed. Let $C_1 < C_2 < \dots < C_n$ be a sequence of random variables that physi-

cally represents the size of a fatigue crack at successive stages of its growth. Then the crack growth at stage j , $C_j - C_{j-1}$, is randomly proportional to the size of the crack, C_{j-1} , and that the specimen fails when the crack size reaches C_n , i.e.,

$$C_j - C_{j-1} = \varepsilon_j C_{j-1} \quad (\text{A.37})$$

where $\{\varepsilon_j\}$ is a set of mutually independent and identically distributed random variables and is also independent of $\{C_j\}$. Then eq. (A.37) reduces to

$$C_j = C_{j-1}(1 + \varepsilon_j) \quad (\text{A.38})$$

This relation leads to the failure condition as

$$C_n = C_o \prod_{j=1}^n (1 + \varepsilon_j) \quad (\text{A.39})$$

where C_o represents the initial flaw size. If the absolute value of ε_j is much less than 1, eq. (A.39) can be approximated by Taylor's expansion such that

$$\ln C_n = \ln C_o + \sum_{j=1}^n \varepsilon_j \quad (\text{A.40})$$

Hence, $\ln C_n$ is normally distributed due to the additive property of the distribution (central limit theorem).

A.3.3 Log-normal probability paper

Log-normal probability paper is similar to normal probability paper, but uses a logarithmic scale to plot the values of the variables. When the data is plotted on the log-normal probability paper and fitted to a straight line, the intercept of 50% probability and slope of the line provides the t_{50} and shape parameter σ , respectively. The shape parameter can be approximated as

$$\sigma \approx \ln\left(\frac{T_{50}}{T_{16}}\right) = \ln\left(\frac{T_{84}}{T_{50}}\right) \quad (\text{A.41})$$

A.4 Extreme value distributions

The largest or smallest order of statistics of a sample is often the relevant inference function in engineering applications of statistics. For example, Al interconnects in semiconductor devices fail at the weakest failure units among many others and, thus, the distribution of lifetime of Al interconnects in semiconductor device is the smallest extreme of the original lifetime distribution of failure units. Hence, the first order statistics defined in eq. (A.18) is correspond to the minimum extreme value distribution of minimum. Similarly, when only the largest values are concerned, the distribution will be determined by the maximum extreme value distribution, i.e., n^{th} order statistics defined in eq. (A.16).

When the number of samples n in eq. (A.16) and eq. (A.18) is large, there may exist an asymptotic distribution; there are three types of asymptotic distributions which can be used to model the extreme value of the interest: type I, type II and type III.

A.4.1 Types of extreme value asymptote

Type I: The type I extreme value model arises from initial distributions that are *unbounded* in the direction of the extreme value, provided that the relevant tail of the initial p.d.f. $f(x)$ decreases at least as rapidly as an exponential function. From this condition it follows that the maximum extreme value from a normal and log-normal distribution can be modeled by a type I asymptote of maxima. The normal distribution is also unbounded at the lower distribution end, so that the minimum extreme of a normal distribution is modeled by a type I asymptote of minima. However, normal distribution can not be justified in the negative domain when the physical variables are concerned, then the minimum extreme asymptote of normal distribution is meaningless in real statistics.

Type II: A type II extreme Value asymptote arises from initial distributions that do not

possess finite moment. In the applied sciences, a distribution without finite moments is difficult to find, and, therefore, it is not considered in this section.

Type III: The type III asymptote arises when an extreme value is considered from an initial distribution $F(x)$ that is bounded in the direction of the extreme value. The minimum value of log-normal distribution can be modeled as this type of asymptote. The minimum distribution of type III extreme is often called Weibull distribution.

A.4.2 Example: Type I extreme value asymptote

Since the distribution of extreme value asymptote is well discussed in various texts of statistics, the maxima of the type I asymptote is discussed in this section as an example.

The characteristic largest value: Consider a sample size of n from an initial distribution $F(x)$. The probability of obtaining one observation that is larger than a value x is

$$\Pr(X \geq x) = 1 - F(x) \quad (\text{A.42})$$

Hence in a sample of size n one would expect, on the average, $n(1-F(x))$ observations larger than x . These observations are often called "exceedances of x ".

The value of x that has, on the average, only one exceedance in a sample of size n is termed the "characteristic largest value u_n " and is defined by

$$1 - F(u_n) = \frac{1}{n} \quad (\text{A.43})$$

Eq. (A.43) represents the tail area of the initial distribution $f(x)$, above u_n , is equivalent $1/n$.

The Type I asymptote of maxima: Consider the largest observation X_n in a sample of size n from an initial distribution $F(x)$. The exact distribution of X_n is given by

eq. (A.16):

$$G_n(x; n) = [F(x)]^n \quad (\text{A.44})$$

If the initial distribution has an unbounded value in the direction of extreme, it must be of the form

$$F(x) = 1 - \exp\{-a(x)\}. \quad (\text{A.45})$$

When $x = u_n$, eq. (A.46) must be connected to eq. (A.43), so that

$$F(x) = 1 - \frac{1}{n} \exp\{a(u_n) - a(x)\}. \quad (\text{A.46})$$

Combining eq. (46) and eq. (44) gives the exact distribution of the largest order statistics X_n from an initial distribution of the form eq. (A.45), in the neighborhood of the characteristic largest value u_n :

$$G_n(x; n) = [1 - \frac{1}{n} \exp\{a(u_n) - a(x)\}]^n \quad (\text{A.47})$$

As the size of n increases, the n^{th} -order statistics X_n increases and so does the characteristic largest value u_n . For large n , the asymptotic distribution of X_n is

$$F(x_e) = \lim_{n \rightarrow \infty} G_n(x; n) = \exp\{-\exp[a(u_n) - a(x_e)]\} \quad (\text{A.48})$$

An analysis, in which the term $\{a(u_n) - a(x_e)\}$ is linearly approximated, shows that eq. (A.49) reduces to

$$F(x_e) = \exp\{-\exp\{-a'(u_n)(x_e - u_n)\}\} \quad (\text{A.49})$$

Here $a'(u_n)$ and u_n are functions of initial sample size n . The quantity $a'(u_n)$ physically represent a scale factor, whereas u_n is a location factor. Expressing $a'(u_n)$ and u_n as $a'(u_n) = 1/\sigma$ and $u_n = \mu$, the type I asymptote is written

$$F_{\max}(x_e; \mu, \sigma) = \exp\{-\exp\{-\frac{(x_e - \mu)}{\sigma}\}\} \quad (\text{A.50})$$

Therefore, the extreme value p.d.f. is obtained by differentiating eq. (A.50):

$$f_{\max}(x_e; \mu, \sigma) = \frac{1}{\sigma} \exp\left\{-\frac{x_e - \mu}{\sigma} - \exp\left\{-\frac{(x_e - \mu)}{\sigma}\right\}\right\} \quad (\text{A.51})$$

The type I asymptote for the largest extremes is related to the type I asymptote for the smallest extremes. For any sample size n , it is true that

$$\min_i \{x_i\} = -\max_i \{-x_i\} \quad (\text{A.52})$$

Hence, the type I asymptote of minimum values is the mirror image of the type I asymptote of maximum value.

The similar method can be applied to type II and type III extreme distributions, and the type and expression of each distribution is summarized in Table 1, in which σ and μ are changed to α and γ to emphasis that they are scale and location factors not the mean and standard deviation.

Table A.1 Distribution functions for the extreme value distributions

Extreme value distribution of the smallest	
Type I	$F(x) = 1 - \exp\{-\exp(\frac{x-\gamma}{\alpha})\}, -\infty < x < \infty$ $f(x) = \frac{1}{\alpha} \exp\{\frac{x-\gamma}{\alpha} - \exp(\frac{x-\gamma}{\alpha})\}$
Type II	$F(x) = 1 - \exp\{-(-\frac{x-\gamma}{\alpha})^{-\beta}\}, -\infty < x < 0$ $f(x) = \frac{\beta}{\alpha} \{-(-\frac{x-\gamma}{\alpha})^{-\beta}\}(-\frac{x-\gamma}{\alpha})^{-\beta-1}$
Type III	$F(x) = 1 - \exp\{-(-\frac{x-\gamma}{\alpha})^{\beta}\}, 0 < x < \infty$ $f(x) = \frac{\beta}{\alpha} (\frac{x-\gamma}{\alpha})^{\beta-1} \exp\{-(-\frac{x-\gamma}{\alpha})^{\beta}\}$
Extreme value distribution of the largest	
Type I	$F(x) = \exp\{-\exp(-\frac{x-\gamma}{\alpha})\}, -\infty < x < \infty$ $f(x) = \frac{1}{\alpha} \exp\{-\frac{x-\gamma}{\alpha} - \exp(-\frac{x-\gamma}{\alpha})\}$
Type II	$F(x) = \exp\{-\frac{x-\gamma}{\alpha}\}, 0 < x < \infty$ $f(x) = \frac{\beta}{\alpha} \{-\frac{x-\gamma}{\alpha}\}(-\frac{x-\gamma}{\alpha})^{-\beta-1}$
Type III	$F(x) = \exp\{-(-\frac{x-\gamma}{\alpha})^{\beta}\}, -\infty < x < 0$ $f(x) = \frac{\beta}{\alpha} (-\frac{x-\gamma}{\alpha})^{\beta-1} \exp\{-(-\frac{x-\gamma}{\alpha})^{\beta}\}$

APPENDIX B

THE EFFECTS OF STRESS IN THIN FILMS

B.1 The origin of stress

A residual stress can be induced in Al thin films by thermal expansion mismatch between the film and the substrate material [163, 164]. A simple example can be given by considering the one-dimensional approximation; if we neglect plastic deformation in the substrate and Poisson's effect, the thermal stress σ_{th} can be given as

$$\sigma_{th} = E_f(\alpha_f - \alpha_s)\Delta T \quad (B.1)$$

where E_f is the Young's modulus of the film, α_f and α_s are thermal expansion coefficients for the film and substrate, and ΔT is the temperature difference. If films are deposited at room temperature, there would not be any residual stress. On the other hand, if films are deposited at higher temperature, thermal stress develops in thin films as they are cooled down to room temperature. The same effect can be expected when films are sintered at high temperature after deposition, which is common in the actual device fabrication process; Al thin films experience several thermal cycle before the completion of device fabrication, such as sintering of films and deposition of passivation layer [165]. The variation of thermal stress in thin films after deposition and during heat treatment is schematically shown in Fig. B.1. In this figure, the stress development during a thermal cycle in films deposited at room temperature are compared with that induced during cooling of films deposited at sintering temperature. For the films deposited at room temperature, compressive stress is induced during heating until the temperature reaches the grain growth temperature where the compressive stress can be released. The compressive stress can be also released through the formation of annealing hillocks. During cooling,

the residual compressive stress is further released by the induced tensile stress, and eventually films experience tensile stress. At the yield stress, a film deforms plastically, and a residual tensile stress remains; the induced stress during cooling of samples deposited at high temperature shows basically the same variation of stress as this except for the amount of plastic deformation. When both films are heat cycled again, then stress evolves from tensile to compressive stress during heating, and compressive and tensile during cooling.

Fig. B.1 A schematic illustration of the thermally induced stress in thin films during heat cycle.

The development of stress in thin films influences the physical properties of the film in two ways. First, the residual tensile stress can induce voids in interconnects. Secondly, the stored energy that was produced during thermal cycle can promote the polygonarization or recrystallization of film structure.

B.2 Stress induced voiding in Al interconnects

Since 1984 it has been observed that voids form in Al interconnects under a passivation layer, even under zero current density [168-178]. Since there is mechanical constraint in unpassivated interconnects, no stress voiding has been reported so far in the unpassivated lines. The void formation becomes more intensive as the induced stress and the thickness of the passivation layer increases, and as the effective linewidth decreases.

The mechanism for void formation is known to be due to the diffusional creep induced by the stress in the interconnects; as a response to the stress, atoms redistribute themselves in the direction where the stress can be relaxed, and this process produce a vacancy flux. The vacancies can accumulate at the vacancy sink, forming a void. The voids formed in narrow interconnects are often found to be transgranular slit-like, while wedge shape voids are more frequent in wider interconnects. It should be noted that the stress voiding in Al interconnects is not necessarily accelerated at elevated temperatures because the tensile stress induced in films decreases as temperature increases. Usually, the film is stress free when the substrate temperature is around 300°C. The morphology of voids in narrow interconnects seems similar to the slit-void forming during electromigration test. Since the electromigration test is usually performed at 200-300°C, the slit void formed during electromigration should not be directly related to the inherent stress in thin films.

Several methods have been proposed to reduce stress-induced void formation: the addition of alloying elements and the an irradiation of passivation layer. The addition of alloying elements is believed to retard the vacancy diffusion, resulting in strengthening effect, and, hence, it can retard the formation of diffusion void; Cu and Pd is such element [147, 175]. The reduction of inherent stress in passivation layer also can reduce the formation of stress induced void, which can be achieved by an irradiation of PECVD SiN

films with mercury light [169] Stress-induced void formation is a problem as serious as electromigration-induced failure, and more investigation is certainly required to control the problem.

B.3 Recrystallization in thin films

B.3.1 Stored energy

As shown in Fig. B.1, when Al thin films are heat cycled, or heat treated, the films are plastically deformed, accumulating stored mechanical energy in films. The evidence of plastic deformation in Al thin films by the thermal stress is shown in Fig. B.2: the slip lines found in samples deposited under the planarizing condition (Fig. B.2.A), and that of RTA heat treated of sample A (Fig. B.2.B). Since the plastic deformation of these films is mainly due to dislocation slip on crystallographic slip system, the passage of dislocations is visible as a line after deformation under TEM. The major slip system for dislocation in an Al crystal is on (111) plane in the [110] direction; each slip direction has a 60° angle. As shown in the figures, the observed slip lines have an intersect angle that is close to 60° . The smaller angle in Fig. B.2.A is due to the curvature of the film surface. The formation of slip lines is very common in deformed materials; the slip lines found in 304 stainless steel after 15% deformation is shown in Fig. B.3. The slip system in 304 stainless steel is the same as in Al because their crystal structures are the same, i.e., FCC. It can be seen that the intersect angle is close to 60° , and the spacing between slip lines is comparable to the that Fig. B.2.A. Thus, it can be qualitatively concluded that the plastic deformation in the films by thermal stress is substantial, at least more than 10% deformation in heat treated samples used in this study.

The quantitative measure of plastic deformation in thin films can be obtained by counting the density of slip lines after thermal cycle; however, it is usually difficult due to the unstable image of slip lines. The slip line is visible under TEM due to contrast in

Fig. B.2 TEM micrographs showing slip lines formed during plastic deformation during cooling after (A) deposition under the planarizing condition and (B) RTA heat treatment. (XBB 933-1216)

Fig. B.3 The image of slip lines found in 304 stainless steel after 15% deformation. (XBB 933-1217)

the residual strain field or a surface layer of oxide formed after the dislocation glide. Since this contrast is very small and unstable, the image gradually disappears during TEM characterization due to local heating by electron beam [180]; it usually took 1 to 2 minutes. In order to quantify the plastic deformation through slip line analysis, the above problem must be avoided. The next following steps can be recommended:

- 1) Obtain the $[110]$ zone axis using a one grain at high magnification. The slip lines in this grain will be lost, while those in other grains are protected. The best crystallographic orientation of the film to obtain the slip line image is around $[110]$ zone axis, because the displacement vector of slip lines is on the $[110]$ direction. Only two sets of slip lines are visible at a given zone axis; the slip lines that are perpendicular to the beam direction are not visible (see Figs. C.2-3).

2) When the zone axis is obtained, decrease the magnification and spread the electron beam. Under this condition, the slip lines in other grains that have similar crystallographic orientation as the characterized grain show the slip lines. Take slip line images in those grains at a condition that the exposure time is the minimum.

B.3.2 Recrystallization

The formation of slip lines in thin films indicates that the thin film underwent plastic deformation during cooling after heat treatment. This plastic deformation increases the stored energy in films. It is well known that the energy stored by deformation can be reduced by polygonalization or recrystallization by either reducing dislocation density or creating dislocation free grain [181]. Both of mechanisms result in the decrease of the grain size. Hence, when samples are heated after deformation, the grain size decreases until the reduction in stored energy is balanced with the increase of the energy by increasing grain boundary density: after recrystallization, normal grain growth driven by grain boundary energy is dominating.

The rate of recrystallization is a function of the amount of stored energy, the heating temperature and the time. The relative importance of those factors requires intensive investigation to understand the recrystallization mechanism in thin films; however, in this study, an attempt was made to qualitatively characterize the recrystallization in thin films. The main goal of this section is to show that recrystallization occurs even in thin films, which has not been studied before. In order to show that the grain size actually decreases with the heat treatment (see Table 3.1) due to recrystallization, the grain size variation must be measured after each successive treatment. However, if the grain size variation is relatively small such that it is within error bound of measurements, which is the usual case, the conclusion can not be decisive. On the other hand, the decay kinet-

ics of the resistivity can be used to monitor the grain size change by heat treatment. As introduced in chapter 3, the kinetics of the resistivity decay is sensitively influenced by grain size and distribution; it provides a good measure for the relative change of the grain size, if the initial condition of solute in films is the same.

In order to investigate the grain size change with the heat treatment, the single line test structure with 6 μm width of the samples deposited at room temperature and deposited under the planarizing temperature were placed in furnace, and they are RTA heat heated at 500°C for 1 minute, followed by water quenching. The decay kinetics of the resistivity were measured at 225°C. Then, these samples are again RTA heat treated at 500°C for 1 minute and quenched, and the decay was measured at 225°C as before. This cyclic heat treatment was repeated for several times, while the decay kinetics were measured after each step; this is schematically shown in Fig. B.4.

Fig. B.4 The thermal cycle applied to the sample for the recrystallization study. Samples are rapidly heated to 500°C, and then quenched after 1 minute. The resistivity variation of samples were measured at 225°C between each cycle.

Fig. B.5 The normalized decay curve of the test lines after various heating cycles: (A) film deposited under the planarizing condition and (B) film deposited at room temperature.

Since the heat treatment condition at each cycle is the same, any change in the decay kinetics should be from the change in the size of Cu sink, which is predominantly grain boundaries. The measured kinetic factor $\varphi(t)$ for samples after each cycle is shown in Fig. B.5; the scale factor β was not changed by the cyclic heat treatment. First, consider the case of sample deposited under the planarizing condition (Fig. B.5.A). This sample is deposited at 450°C, and, thus, plastic deformation was induced during cooling as can be seen from the slip lines in Fig. B.5.3. As this sample is heat cycled further, the kinetics of the decay becomes faster up to the second cycle. After third cycle, the decay kinetics become about the same as those in the second cycle, although they are slightly slower. There is no significant change in the decay kinetics after the third cycle. On the other hand, the variation of the decay kinetics of the sample deposited at room temperature show a different variation with the cyclic heat treatment (Fig. B.5.B). After the first cycle, the decay kinetics show the unique feature that was discussed in chapter 3; the decay becomes suddenly slower after 90 % of the decay, which is attributed to the bimodal distribution of grain size. Cyclic heat treatment after the first cycle changes the decay kinetics in two ways. First, the initial decay is slower after the heat treatment. However, the later stage of decay becomes faster than the first cycle; the unique decay feature after 90% of the decay found after the first cycle becomes invisible. As a result, the decay curve becomes generally slower and continuous without sudden change in the kinetic curve. As in the sample deposited under the planarizing condition, after the third cycle there is no significant variation in the decay kinetics. One more interesting observation to note is that the decay kinetics of both samples becomes almost the same after third cycle; they show about the same kinetics and curve shape.

It was found that there are two competing forces acting toward microstructural change in this experiment: grain growth and recrystallization. If only the normal grain growth is working at the heat treatment temperature, the decay kinetics should decrease

with heat treatment cycle due to the increase in the grain size. However, heat treatment induces plastic deformation during cooling of the sample, and the resulted stored energy tends to recrystallize the film. Hence, the grain size of the film should be determined by the net of two driving forces:

$$\text{grain size} = -\text{recrystallization} + \text{grain growth} \quad (\text{B.2})$$

Since the temperature and time for the heat treatment is fixed for all cycles, the driving force and the rate of recrystallization is insensitive to the heat cycle; it should be relatively the same for each cycle. On the other hand, the driving force and rate of grain growth is grain size dependent, and, hence, the previous grain size influences the grain growth rate during next heat cycle; grain growth is faster in films with smaller grains.

The sample deposited under the planarizing condition contained relatively large grains; the mean grain size is 2.4 μm . During 1 minute heating of this sample at 500°C, grain growth would not be significant, rather the recrystallization should be predominant. Therefore, the grain size decreases with the first few heat cycles, resulting in a faster decay rate. However, when the reduction of the grain size is big enough to induce a considerable rate of grain growth, the influence of the grain growth can not be ignored. Consequently, there exists a critical cycle after which the grain growth and recrystallization is balanced, and grain size is not changed by the further heat cycles. There is a quasi-steady state grain size after the second cycle. The same analysis can be applied to the case of sample deposited at room temperature. In the as deposited condition, the film contains extremely small grains, less than 0.4 μm in diameter. Also, there is no plastic deformation and thus no driving force for recrystallization. Upon heating at 500°C for 1 minute, an extensive amount of abnormal grain growth occurs, producing a bimodal distribution of grain size; the bimodal distribution of grain size results in the unique feature of decay kinetics as discussed above. During cooling of this sample, film experience the tensile stress as shown in Fig. B.1, resulting in accumulation of stored energy. In the

second cycle, the stored energy tends to recrystallize the film, but this is overwhelmed by the grain growth rate due to small grains. However, the driving force for the recrystallization is effective on a few large grains in the films, making those grains smaller. Thus, the grain size generally increases, while the distribution becomes uniform by eliminating a few large grains; this explains the reason why the decay kinetics becomes slower after the heat cycle, while the later stage of the decay kinetics becomes faster. As grain size increases, the rate of grain growth decreases and reaches the point at which it is balanced by the recrystallization; this occurs at the third cycle. Qualitatively, the critical condition for films where the rate of grain growth and recrystallization is balanced should not be influenced by the initial grain structure, and, therefore, the grain size and its distribution after critical heat cycle should be the similar for each sample; the decay kinetics of each sample after fourth cycle is relatively the same.

The analysis shown here is qualitative but it proves that recrystallization actually happens even in thin films, although grain size reduction by the recrystallization is not substantial compared to that in bulk materials. Since the grains in thin films is extremely small compared to the bulk materials, grain growth can easily overwhelm the recrystallization during heating. It was possible to detect the grain size reduction by recrystallization in this study because the heating was done for only 1 minute, and grain growth was presumably retarded by grain boundary drag by the Cu or grain boundary pinning by the film surface; these factors made the recrystallization more significant. If pure Al thin films with wider linewidth are tested, or heating time is longer than 1 minute, the recrystallization of films can not be easily observed; this is probably the reason why only grain growth of films is observed in the conventional studies, in which films are heat treated at least 30 minutes. It appears that the phenomenon of recrystallization is not technically important. However, the growing tendency to deposit films under planarizing conditions as used in this investigation and to use RTA heat treatment for the device fabrication does

increase the potential importance of the recrystallization of films. The several heat cycles that the interconnects usually experience during device fabrication would reduce the grain size, if films are heated for a short period of time to minimize the undesirable diffusion problem. In this case, the electromigration failure statistics would be changed accordingly, which must be taken into account. The systematic study of recrystallization of thin films is highly recommended for technical importance, as well as scientific interest.

APPENDIX C

THE ELECTRICAL RESISTIVITY OF DILUTE ALLOYS

Since an impurity atom acts as a scattering center for electrons, the electrical resistivity of a sample is increased by the presence of impurity atoms, and the relation is expressed as

$$\rho = \rho_o + kC \quad (\text{C.1})$$

where ρ_o and k denote the resistivity of pure metal and the correlation constant, respectively. This is known as Matthiessen's rule [125]. This rule is valid as long as impurity atoms are uniformly distributed throughout the sample; however, when the sample has a non-uniform distribution of impurity atoms, a modification is necessary. Although eq. (C.1) can not represent the electrical resistivity of a whole sample, it should hold its validity at least locally. Now, consider the sample geometry shown in Fig. C.1. The local resistance in a unit volume $dx dy dz$ is

$$\partial R(x, y, z) = \rho(x, y, z) \frac{dx}{dy dz} = (\rho_o + kC(x, y, z)) \frac{dx}{dy dz} \quad (\text{C.2})$$

The local resistance combines according to the law of parallel conductors to give the resistance of the yz plane at position x with the length of dx , $\delta R_{yz}(x)$, and it becomes

$$\frac{1}{\partial R_{yz}(x)} = \int_0^w \int_0^T \frac{dy dz}{\rho(x, y, z) dx} \quad (\text{C.3})$$

and

$$\partial R_{yz}(x) = \rho_o \left[\int_0^w \int_0^T \frac{1}{1 + \frac{k}{\rho_o} C(x, y, z)} dy dz \right]^{-1} \quad (\text{C.4})$$

Fig. C.1 A graphic illustration of the sample geometry for the construction of the electrical resistivity

Since the serial connection of conductor is established along the x direction, the total resistance becomes

$$R = \rho_T \frac{L}{TW} = \int_0^L \partial R_{yz}(x) \quad (C.5)$$

From eq. (C.4) and (C.5) the total resistivity of the sample is

$$\rho_T = \rho_0 \frac{TW}{L} \int_0^L \left[\int_0^W \int_0^T \frac{1}{1 + \frac{k}{\rho_0} C(x, y, z)} dy dz \right]^{-1} dx \quad (C.6)$$

Substituting Lu , Wv and Tw for x , y and z where u , v and w denote the normalized coordinates of the x , y and z axis, eq. (C.6) becomes in dimensionless form

$$\rho_T = \rho_0 \int_0^1 \left[\int_0^1 \int_0^1 \frac{1}{1 + \frac{k}{\rho_0} C(u, v, w)} dv dw \right]^{-1} du \quad (C.7)$$

Since $C(u, v, w) \leq 1$, the integral with respect to v and w can be performed as a geometric series [115]:

$$\begin{aligned} \left[\int_0^1 \int_0^1 \frac{1}{1 + \frac{k}{\rho_0} C(u, v, w)} dv dw \right]^{-1} &= 1 + \left(\frac{k}{\rho_0} \right) \chi_1 + \left(\frac{k}{\rho_0} \right)^2 (\chi_1^2 - \chi_2) \\ &\quad + \left(\frac{k}{\rho_0} \right)^3 (\chi_1^3 - 2\chi_1\chi_2 + \chi_3) + \dots \end{aligned} \quad (C.8)$$

where χ_n is the integral of the n th power of $C(u,v,w)$ with respect to v and w . Since the value k/ρ_o is generally small for most impurities, eq. (C.8) can be approximated by the first two terms when the concentration of solute atoms are small enough. Therefore, the total resistivity of the sample becomes

$$\rho_T \approx \rho_o + k \int_0^1 \int_0^1 \int_0^1 C(u,v,w) du dv dw \quad (C.9)$$

This result leads to a modified Matthiessen's rule that applies to most dilute alloys, written as

$$\rho \approx \rho_o + k\bar{C} \quad (C.10)$$

where $\bar{C}$ is the mean concentration, or equivalently the total number of electrically active impurities in a sample [117].

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