1 Introduction to Electromigration

Electromigration, or electrotransport, describes the phenomenon of atomic diffusion in metal driven by an electric current. Its study can be traced back more than a century, starting with the first observation reported by Geradin [1] in molten alloys of lead-tin and mercury-sodium. Systematic studies did not start until the early 1950s with the work of Seith and Wever at the University of Muenster, Germany [2]. By measuring the mass transport across the phase diagram of some Hume–Rothery alloys, they observed that the direction of mass transport can be reversed and is correlated with the type of the majority charge carriers, i.e., electrons or holes, in the specific alloy phase. This observation provided the first evidence concerning the nature of the driving force for electromigration. It showed that the atomic motion is not determined solely by the electrostatic force imposed by the applied electric field; instead, it depends on the direction of motion of the charge carriers. This prompted Seith to introduce the idea originated by Skaupy [3] of "electron wind" to account for the induced mass transport, an idea that laid the foundation for the basic understanding of electromigration. Seith and Wever [4] also introduced the method of using the displacement of an indentation on a metal wire to measure the induced mass transport. This "marker motion" technique, now called the vacancy flux method, has become one of the standard measurements of electromigration in bulk metals.

The concept of the "electron wind" driving force was first formulated by Fiks [5] and Huntington and Grone [6]. Working independently, these authors employed a semiclassical "ballistic" approach to treat the collision of the moving atom by the charge carriers. In a more rigorous treatment, Huntington and Grone considered the initial and final quantum states of the charge carriers involved in the collision process, where the "wind" force experienced by the moving atom is derived by integrating the spatial variation of the interaction with the charge carriers. These ideas yielded a driving force depending on the type of defect, the interaction with the charge carriers, and the atomic configuration of the jumping path.

The formulation of the driving force was a major contribution to the study of electromigration, as it demonstrated the possibility of using electromigration to probe the interaction of mobile defects with charge carriers in metals. This has stimulated considerable interest starting in the 1960s in theoretical and experimental studies on electromigration in metals. In theoretical studies, Bosvieux and Friedel [7] developed the first quantum mechanical formulation of the driving force in terms of electron–ion interactions for a simple case of impurity atoms in a "jellium." With some simple

2 1 Introduction to Electromigration

model assumptions, these authors have formulated an approach that can be extended to metals with more complex electronic structures. This has stimulated a series of subsequent theoretical studies with focus on the physical basis of the driving force, particularly regarding the dynamic screening of the moving ion and the effect of the band structure on the electron–ion scattering. (See reviews by Verbruggen [8] and Sorbello [9].) While the theory continued to develop, experimental data have accumulated to show systematic trends to collaborate the theoretical results. In the experimental studies, the interest was initially concentrated on self-electromigration in pure metals using primarily the vacancy flux method and with a few using radioactive isotopes. These studies were first focused on metals with electron charge carriers and then extended to metals with hole carriers (see the reviews by Huntington [10]). The experimental study was later extended to alloys and liquid metals by Rigney [11].

Until that time, the application of electromigration (EM) was rather limited, with efforts largely directed toward the purification of interstitial, particularly gaseous, impurities in refractory metals [12]. The interest and the direction of electromigration study took a drastic turn in 1966 when Blech and Sello [13] reported that the crack formation in aluminum conductor lines on silicon chips was induced by electromigration. This was a serious reliability problem for the microelectronics industry, coming at a time when the microelectronics industry was starting the development of verylarge-scale integration (VLSI) of integrated circuits [14]. This has generated significant interest to study electromigration, not only for its basic physics, but as an important reliability problem for the integrated circuits. Most of the studies were aimed at electromigration in thin film conductors used for multilevel on-chip interconnects with linewidths of submillimeters and operated at moderate temperatures of about half the absolute melting point. Under these conditions, the current density driving the mass transport increases by more than two orders of magnitude, while electromigration occurs primarily along structural defects, such as surfaces, interfaces, and grain boundaries. Particularly relevant to damage formation is the flux divergence site where damages in the form of voids or hillocks can form because of the local imbalance of atomic flux induced by material and microstructure inhomogeneity. Such characteristics of EM damage have shifted the focus of the investigations from bulk materials to thin films and conductor lines [15–17].

Until the early 1990s, interest in EM was primarily focused on aluminum lines, the dominant material used for on-chip interconnects at that time. As the technology evolved, the Al on-chip interconnects became more complex with multiple metal levels integrated with $SiO₂$ interlayered dielectrics. Following Moore's law [18], device scaling continues to reduce the size of the conductor lines by a factor of ~ 0.7 every technology generation, with corresponding increase in its number to sustain the improvement of device density and chip performance. This cumulated to the development of $A\text{VSiO}_2$ interconnects with 5–6 metal levels and a minimum linewidth of ~0.4 µm for high-performance microprocessors of the 0.25 µm technology node. At this time, the study of electromigration has advanced well into the microscale domain with materials and microstructure characteristics distinctly different from bulk metals or thin films.

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One distinct aspect of EM in conductor lines arises from the thermal stresses generated in the line due to the confinement by the Si substrate and the interlevel dielectrics and barriers to contain the metal line. The thermal stress provides an additional driving force to counter the electrical current for mass transport and can substantially affect the kinetics and mechanism for damage formation. The stress effect on EM was first observed by Blech in 1976 in a study of EM in Al conductor lines [19] and established the concept of a critical current density-length (jLc) product with a "critical length" Lc where the stress gradient can completely counteract the current j driving force to stop EM [20, 21]. The stress effect took a drastic turn in the 1980s to become an important reliability problem with the finding of stress-induced void formation in passivated Al lines that can cause line failure without EM [22, 23]. This phenomenon has generated great interest at that time to investigate the thermal stress characteristics and the stress voiding phenomenon. It soon became clear that stress voiding is synergetic to electromigration, and together they form a framework for analyzing the kinetics of damage formation under EM. This has led to the formulation of the Korhonen equation [24, 25] and subsequently more general 3D analyses.

This can be considered the first major period of EM studies on conductor lines driven by technological needs to develop Al-based on-chip interconnects for largescale integration. Significant interest has been generated from the industry and university laboratories with research topics focusing on effects of materials, microstructure, and line dimensions on mass transport and the development of reliable EM structures. These included the solute effect [15], the intermetallic layer effect [26], and the development of statistical studies [27], among others.

Since then, the study of electromigration has been sustained by unprecedented advances of the IC miniaturization from the micro- to the nanoscale, with continuing improvement of the device density, chip performance, and manufacturing cost as predicted by Moore's law. This has prompted the development of Cu interconnects to replace Al interconnects in 1997 [28]. and subsequently the implementation of low *k* dielectrics as interlevel dielectrics [29]. The development of Cu damascene structures brought new focus into the study of EM and thermal stresses in Cu interconnects. This began the second major period of electromigration studies where not only the basic material set has changed but also the interconnect structure with the development of the dual damascene process for Cu interconnects [30]. While Cu has better intrinsic reliability than Al, electromigration continued to be a major reliability concern with distinct characteristics and damage mechanisms. The degradation of EM reliability for Cu damascene lines depends on materials and processing, particularly relating to defects induced by chemical-mechanical polishing (CMP) at the interface and the plasma processing of the weak low *k* dielectrics. Several important studies have been reported, including the analysis by Lane et al. showing that the activation energy for void growth under EM can be directly correlated to the bond energy of the Cu interface [31]. Also important was the prediction by Hu et al. that the EM lifetime would degrade by half for every technology node due to dimensional scaling even with a constant current density [32]. Results of these studies clearly showed that

4 1 Introduction to Electromigration

interfacial engineering is an effective approach for improving the EM reliability for Cu damascene interconnects. This has led to several approaches to improve EM reliability for Cu metallization, including metal cap layers [33] and solute alloying [34], among others.

With continued scaling, the dimensions of the Cu lines reach to the nanoscale, which significantly increases the number and complexity of the interconnects together with changes in the Cu microstructure and increases in the line resistivity. Responding to the technological needs, the EM studies of Cu damascene structures were extended to the nanoscale and the development of alternate metallization. These included the formulation of general 3D kinetic analyses [35, 36], the development of statistical tests at a massive scale [37, 38], the scaling effect on microstructure [39, 40], and electrical resistivity [41, 42].

This book aims to provide a comprehensive review of the current understanding of electromigration and interconnect reliability from fundamentals to nanointerconnects. It is organized into nine chapters and largely follows the chronological order of electromigration studies, starting from the basic studies in metals and extending to interconnects from the microscale to the nanoscale. First, the fundamentals of electromigration and the studies of bulk metals are reviewed in Chapter 2, including a formulation of electromigration based on irreversible thermodynamics, a kinetic analysis of the solute effect and a review of the theory and bulk materials studies. In Chapter 3, the discussion on EM in metal lines starts with thermal stresses induced by dielectric and substrate confinement with distinctive characteristics to interact with EM to control the mass transport and void formation. Here we describe the X-ray diffraction technique used to determine the triaxial stress state in Al and Cu lines and show how the structural confinement can give rise to substantial hydrostatic stresses to induce void formation leading to line failure. This is followed by Chapter 4 analyzing the kinetics of mass transport under EM and thermal stresses leading to the Korhonen equation and the Blech "short-length" effect. Here analytical solutions and simulations are presented in 1D to analyze the microstructure and stress effects on damage formation and early failures under EM.

Starting from Chapter 5, the discussion is focused on EM in Cu interconnects and topics related to the scaling effects at nanoscale, including microstructure evolution, electrical resistivity, massive-scale statistical tests, and power grid applications. The discussion proceeds first in Chapter 5 on EM characteristics and reliability studies of Cu conductor lines as scaling continues to the nanoscale for ultra large-scale integration (ULSI). The Cu interconnects fabricated by the dual damascene process have structural features leading to mass transport and failure mechanisms distinctly different from the Al interconnects. Several innovative approaches have been developed to improve EM reliability for Cu interconnects, including the use of cap layers and alloying effects, which will be discussed. In Chapter 6, we investigate the scaling effect on microstructure evolution and the implication on EM reliability of Cu and Co interconnects. The scaling effect on microstructure was measured using a highresolution transmission electron microscopy (TEM)-based precession electron diffraction (PED) technique. With this technique, microstructure evolution was measured to

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22 nm linewidth for Cu interconnects and to 26 nm linewidth for Co interconnects. Based on the PED results, Monte Carlo simulation was developed based on total energy minimization to project the scaling effect on grain growth and EM reliability for future technology nodes.

In Chapter 7, the analysis of EM and stress evolution is generalized from 1D to 3D damascene interconnects. This chapter starts with a general 3D analysis of stress evolution by treating the vacancies and displaced atoms generated under EM as local volumetric strains in the grain interior and at grain boundaries (GBs). Then a physicsbased simulation is set up to analyze the microstructure effects on stress evolution and void formation, considering the variations of the GB diffusivities and elastic properties of individual grains in the interconnect. Results from the simulation are combined with scanning and transmission electron microscopies to study void nucleation, migration, growth, and shape evolution, leading to interconnect degradation.

With continued scaling to the nanoscale, the statistical nature of damage formation becomes important to assess EM reliability, which is dominated by the early failures of the weakest links. This topic is discussed in Chapter 8, presenting a novel approach based on the Wheatstone Bridge technique to perform statistical EM tests at a massive scale to detect early failures in very large systems. In contrast, we show in Chapter 9 that recent measurements showed that the weak link approach cannot accurately predict the lifetime for power grid–like structures. A novel approach is presented for power grid EM assessment using a physics-based approach combined with a mesh model to account for redundancy while still fast enough to be practically useful. Existing physical models for EM in metal branches are extended to track EM degradation in multibranch interconnect trees across the die. These problems are important for future development of reliable Cu interconnects as scaling continues to expand the wiring structure to the material limit at the nanoscale.

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2 Fundamentals of Electromigration

2.1 Introduction

In this chapter, a formal description of electromigration is presented by treating electromigration as a phenomenon of mass transport under a driving force in metals within the framework of irreversible thermodynamics. Although the formulation as presented is formal, it is useful in clarifying the thermodynamic nature of electromigration as arising from the interaction of the moving atoms and the charge carriers. Following this formulation, an example is given to describe electromigration in dilute alloys as a correlated atomic diffusion phenomenon, which is used to analyze the solute effect on electromigration in Section 2.3. This example shows that by considering the details of the correlation in the atomic jumping process, the thermodynamic parameters can be expressed in terms of the atomic jumping frequencies and the correlation between the solute and the solvent atoms. In this way, the solute effect on electromigration can be formulated and analyzed with results to show how the solute diffusion can affect the solvent diffusion in electromigration. In Section 2.4, the theory on the driving force is summarized with a discussion on the controversy of the screening effect on the direct force. Then we present the results from experiments designed to measure electromigration of hydrogen impurities to resolve this question. This is followed by reviewing in Section 2.5 the EM studies carried out in two systems of bulk metals: substitutional and interstitial. The chapter then concludes with a summary.

2.2 Thermodynamic Description of Electromigration

Electromigration can be treated as a general phenomenon of forced atomic motion in a solid with several interacting components within the framework of irreversible thermodynamics (see, for example Adda and Philibert [1]). Here we follow the approach of Huntington [2] to study the solute effect on electromigration in dilute alloys.

In a multicomponent 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 in general by writing the atomic fluxes J_i as

2.2 Thermodynamic Description of Electromigration 9

$$
J_i = \sum_j L_{ij} X_j \qquad (i = 1, 2, \dots, n), \tag{2.1}
$$

where L_{ij} is the phenomenological coefficient correlating the flux J_i of the *i*th component to the driving force X_i of the *j*th component. In general, the driving force X_j is derived from the gradient of the chemical potential μ_i and other types of potential such as the electrical potential and thermal and stress gradients. In electromigration, the driving forces from the thermal and stress gradients can also be important as discussed in later chapters, depending on the system and the boundary conditions. Here we express the flux equations separately for the motion of the atoms and the charge carriers and assume uniform temperature and stress distributions as follows:

$$
J_i = T^{-1} \sum_j L_{ij} \nabla (\mu_j + q_j \phi) - T^{-1} L_{ie} q_e \nabla \phi,
$$
 (2.2a)

$$
J_e = T^{-1} \sum_j L_{ej} \nabla (\mu_j + q_j \phi) - T^{-1} L_{ee} q_e \nabla \phi.
$$
 (2.2b)

Here the diagonal elements L_{ii} are related to the diffusion of the *i*th element, and L_{ee} is related to the flow of the charge carriers. There are two types of off-diagonal elements: *Lij*, relating to the effect on the atomic jumps of the *i*th element due to the correlated jumps of the *j*th element, and *Lie*, relating to the interaction between the atom and the electrons. The first type of these elements, *Lij*, applies to both the chemical potential μ_j and the electrical potential $q_j \phi$, where the correlation in atomic jumps affects not only the diffusion process relating to μ_j but also the electromigration process relating to $q_i\phi$. The second type of the off-diagonal elements, L_{ie} , constitutes the "electron-wind" force due to the interaction of the charge carriers with the moving ion. This term is usually combined with the direct electrostatic force, i.e., the $q_i \nabla \phi$ term, to yield the electromigration driving force in terms of an effective charge *Z* [∗]*e* as

$$
F_{\text{eff}} = |e|Z^*E
$$

= $|e|(Z^w + Z^e)E,$ (2.3)

where $Z^e eE$ is the electrostatic force and $Z^w eE$ the "electron-wind" force and $|e|$ the absolute value of the electronic charge and *E*, equal to $-\nabla\phi$, is the electric field. In this way, the formulation can analyze the solute effects on electromigration in dilute alloys.

At this point, not all of the nondiagonal coefficients are independent so that the Onsager relation cannot be applied to reduce the number of independent coefficients [2]. Before this simplification is carried out, the mass conservation condition $\sum J_i = 0$ and the mechanical equilibrium condition $\sum \nabla (\mu_j + q_i \phi) = 0$ can be imposed to ensure an equilibrium state of the system. These conditions reduce the number of the independent coefficients L_{ij} . For a system where mass transport involves diffusion via vacancies, it is convenient to introduce the vacancy as an additional component to balance the mass transport of the moving atoms as

10 2 Fundamentals of Electromigration

$$
J_{\nu} = -\sum_{i} J_{i}.\tag{2.4}
$$

Using this condition, one can transfer (2.2a) and (2.2b) from the laboratory reference frame to a lattice reference frame where the atomic motion can be observed as relative movement of the lattice planes. This approach of tracking the mass transport in electromigration is one of the commonly used methods in measurement and is called the *vacancy flux method* [2], which will be discussed in Section 2.4.

After transposing the flux equation (2.2a) and (2.2b) to the lattice frame, the system is under mechanical equilibrium where the flux and the force are conjugate variables and the Onsager relation can be applied to yield $L_{ij} = L_{ji}$. After this simplification, a basic formalism is established to treat electromigration in multicomponent systems. Several applications of common interest can be found in [2, 3].

2.3 Kinetic Analysis of Solute Effect on EM in Binary Alloys

In this section, the thermodynamic formulation is used to analyze the solute effect on EM in binary alloys [4, 5]. This problem was of considerable interest in the early EM studies since the addition of copper was found to be effective to improve EM lifetime of the aluminum lines [6]. In a dilute alloy, the total atomic flux comes mainly from the diffusion of the solvent atoms, and so to understand the solute effect, one must analyze how the diffusion of the solvent atoms can be affected by the solute atoms and change the overall atomic transport. This problem was first analyzed by Doan [7], who investigated the atomic process in impurity diffusion and derived the various ratios of the jumping frequencies. The solute effect presented here is based on irreversible thermodynamics and analyzing the kinetics to examine how the interactions of the electrons with the solute atoms can affect the transport of the solvent atoms under EM [5]. Once the problem is formulated, the analysis is applied to several alloy systems to evaluate the solute effect and to search for solute additions that can reduce the overall electromigration.

Consider a homogeneous binary alloy of atomic species *a* and *b* with atomic concentrations of *c^a* and *cb*, respectively. Following thermodynamics, the atomic fluxes under an electric field E at temperature T can be related to the driving forces through the phenomenological coefficients L_{ij} as

$$
J_a = -(L_{aa}\nabla\mu_a + L_{ab}\nabla\mu_b)/T + (L_{aa}q_a + L_{ae}q_e + L_{ab}q_b)E/T
$$

\n
$$
J_b = -(L_{bb}\nabla\mu_b + L_{ba}\nabla\mu_a)/T + (L_{ba}q_a + L_{be}q_e + L_{bb}q_b)E/T,
$$
\n(2.5)

and the vacancy flux is

$$
J_{\nu} = -(J_a + J_b). \tag{2.6}
$$

In (2.5), the flux consists of two parts: the first two terms on the right are the diffusion contributions due to the concentration gradients, and the othes are the EM induced by the field *E*. Here μ_a and μ_b are the chemical potentials associated with the