Synopsis

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Title of the thesis: Mass Transport in Cu-Interlayer-Si Systems due to Various Types of Thermo-Electro-Mechanical Excursions

This work falls in general area of the electro-thermo-mechanical driven mass transport in Cu-Si systems, which often finds relevance while accessing reliability issues pertaining to thin film interconnects in microelectronic devices. In such a system, the major driving forces are electric potential gradient (and hence electromigration), current crowding induced temperature gradient (and hence thermomigration) and coefficient of thermal expansion (CTE) mismatch induced stresses. Herein, a coupling between different driving forces, such as electromigration and thermomigration, may also occur, which can subdue or accelerate the mass transport in Cu. In addition, due to an increase in the interface area to volume ratio in very thin interconnects, the contribution of diffusion through the Cu-Si interface in the overall mass transport cannot be neglected. Therefore, it can be inferred that electromigration, thermomigration and thermal stress induced failures of Cu-Si systems should be sensitive to the property of the interface, making it imperative to investigate the role of the interlayer placed in between Cu and Si in mass transport. Accordingly, this work focuses on studying the role of the coupling between the aforementioned major driving forces, especially electric potential gradient and temperature gradient, and the interlayer on the mass transport behavior in Cu-Si system. To improve the life time of devices and improvement of reliability issues it is better to understand these phenomena also from the interface aspect; this idea has been the driving force behind the work taken in this study.

This work focuses on the studying the effects of interlayers on electric current and thermal cycling induced mass transport in Cu thin films. Accordingly, the following are the sub-objectives of this work:

- Studying the role of a bend in Blech structure on current crowding and temperature gradient.
- Understanding the mass transport arising due to electromigration-thermomigration coupling and CTE mismatch induced stresses in Cu thin films deposited on Si substrate
- To study the effect of the interlayer film placed between Cu and the substrate on the mass transport in Cu film under various driving forces (as mentioned in the previous sub-objective)
- Proposal of a roadmap for selection of materials for future highly reliable interconnects and their processing conditions.

Firstly, the effect of current crowding induced temperature gradient on the electric current induced mass transport in Cu films was studied. This effect was studied using samples fabricated according to the standard Blech configuration, wherein long Cu thin film was deposited on Si substrate with very thin W interlayer, and all tests were performed at a constant temperature by passing only one electric current density until the resistance increased by 20 %. In these tests, regular mass transport at the cathode, termed as forward mass transport, was observed along with an anomalous mass depletion at the anode, termed as backward mass transport, especially when currents of very high densities ($>10^6$ A/m^2) was passed (**Figure 1**).

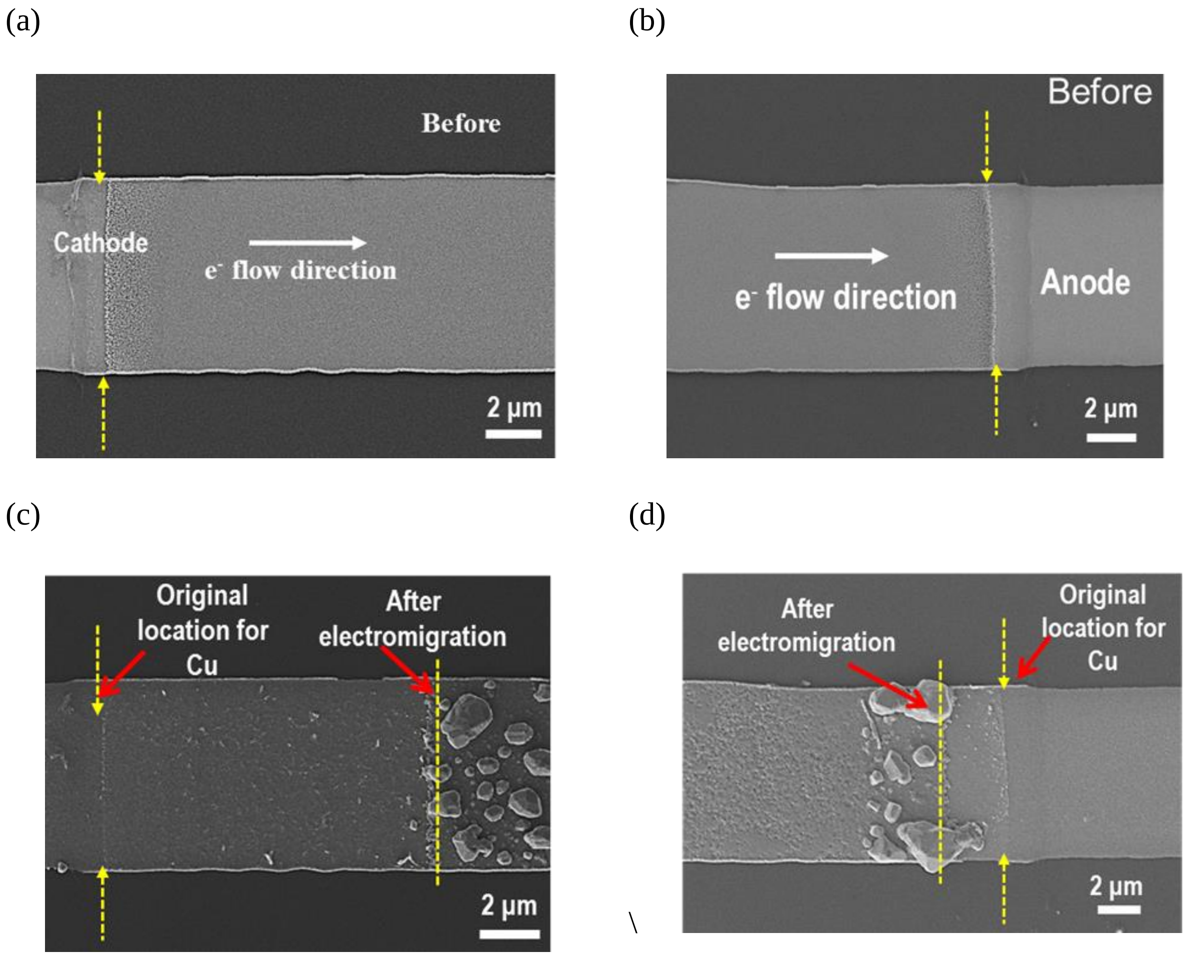


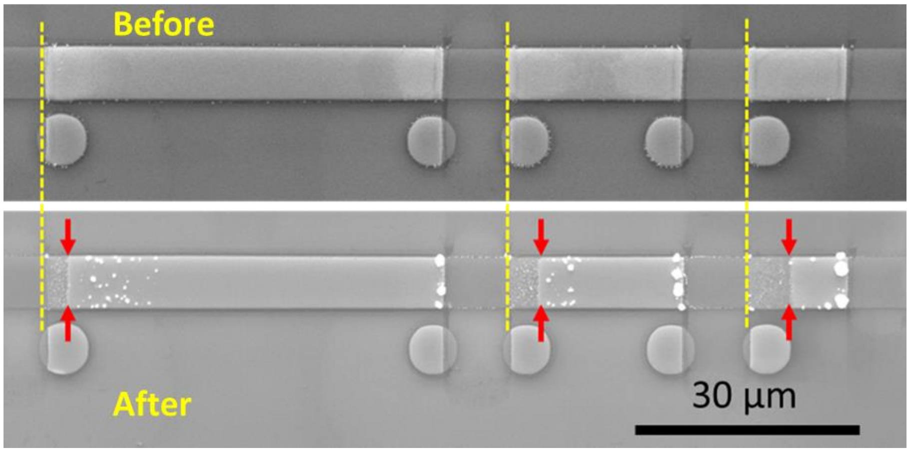
Fig 1. Representative SEM micrographs showing (a) cathode side before electromigration test, (b) anode side before electromigration test, (c) near to the cathode side after electromigration test, and (d) near to the anode side after electromigration test.

The anomalous backward mass transport behavior is explained by illuminating the coupling between the temperature gradient induced mass transport (i.e., thermomigration) and the electric current induced mass transport (i.e., electromigration) at the anode. Herein, temperature gradient was estimated using finite element analysis, performed using COMSOL Multiphysics software, using the full-length scale model. The kinetics of the anomalous backward mass transport at the anode was also studied by varying current density, thickness of interlayer and substrate temperature. The anomalous mass transport, which has origins in the establishment of very high temperature gradients at the anode, became more pronounced with increase in the current density. In addition to the temperature gradient, the temperature of the sample also increased with increase in the current density, and since the kinetics of electromigration as well as thermomigration induced mass transport are diffusion controlled, an increase in the current density further exacerbates the net mass transport, irrespective of whether it is the regular forward or anomalous backward mass transport. *It was observed that the kinetics of the backward mass transport increased with decrease in the interlayer thickness and increase in the current density as well as substrate temperature. However, the current density affects the backward mass transport the most.* A simple design philosophy for reducing the backward mass transport in Cu film near the anode is proposed.

Subsequent to establishment of the existence of significant thermomigration-electromigration coupling in samples fabricated using Blech configuration, systemic experiments were performed to understand the role of the thermomigration-electromigration coupling induced mass transport on the so-called Blech length effect[1]. Herein, experiments were performed by passing current through a sample, wherein a long Cu film on Si substrate with W interlayer was segmented into multiple stripes with lengths varying from 10 μm to 200 μm (see **Fig. 2a** for a micrograph of the sample).

[1] Blech length effect is understood as elimination of electromigration (i.e., material depletion at the cathode and the material accumulation in form of whiskers or hillocks at the cathode) when the product of the current density and the sample length is smaller than a critical value.

(a)



(b)

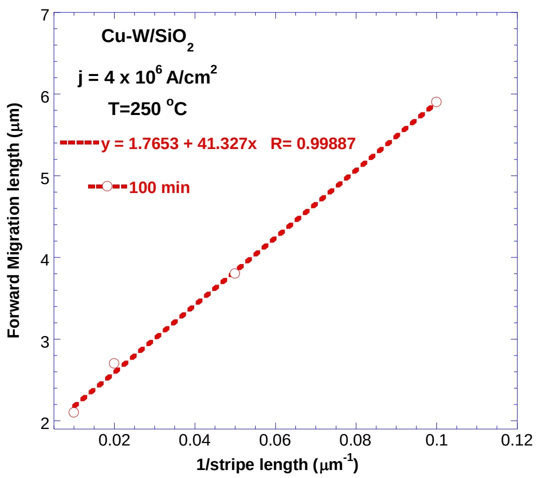


Figure 2: (a) SEM micrograph showing the region near the cathode (i.e., the forward mass transport) of Cu stripes on W interlayer after 100 min of electric current loading. The top and the bottom sets of micrographs show the sample before and after the conclusion of the test. Yellow lines indicate the initial position of Cu stripe, whereas the red arrows indicate the edges of Cu film after the test. Variation of extent of the forward mass transport at the cathode as function of (b) inverse of the stripe length.

Tests were performed up to either a fixed time or the time till the resistance of the entire sample increased by 20%. If the experiments were performed for very long period (e.g., when the resistance increased by 20 %), anomalous backward mass transport at the anode was observed in segmented Cu samples (as shown in **Fig. 1**), whereas if the experiments were performed for much shorter time (e.g., 100 min), then only forward mass transport at the cathode could be observed at lower magnifications (see **Fig. 2a**). Interestingly, contrary to the classic Blech length effect, *the net mass transport at the cathode (i.e., forward mass transport) increased with a decrease in the stripe length when electromigration-thermomigration coupling was significant* (see **Fig. 2b**). We term this behavior as *inverse Blech length effect*. These results imply that thermomigration, besides electromigration, should also be considered while understanding the role of electric current on reliability of Cu-Si systems having bends, e.g., modern 3-D Cu interconnects fabricated using dual Damascene process, etc., as the thermomigration-electromigration coupling violates the conventional wisdoms of mass depletion under the influence of electric current, such as depletion at the cathode only, hillock or whisker formation only at the anode, existence of Blech length effect, etc.

Subsequent to observation of two new phenomena (i.e., anomalous backward mass transport and inverse Blech length effect), role of an interlayer placed in between SiO_2 and Cu on the electromigration-thermomigration coupling induced mass current in Cu film was studied. W, Ta and Ti were selected as interlayers, as they have widely different bonding and intermixing behavior with Cu, with Cu-Ti and Cu-W being the strongest and the weakest in terms of adhesion. *Herein, the Blech length effect was observed when the bonding between the Cu and the interlayer was strong (e.g., for Cu-Ti-Si system)* (see **Figure 3**), *whereas inverse Blech length effect was observed in weakly bonded interfaces (e.g., Cu-Ta, Cu-W, Cu-Ti(O) (see **Figure 4**)).* Therefore, a transition from regular Blech length effect, which is often used as a design paradigm in microelectronic industry, to the inverse Blech length effect can be induced by changing the interfacial layer between Cu and Si (and its deposition condition). The same transition in the observation of anomalous backward mass transport at the anode can also be noted. The interface structure was characterized using transmission electron microscope, and the obtained information, along with the finite element analysis, was used to explain the observed results.

(a) (b)

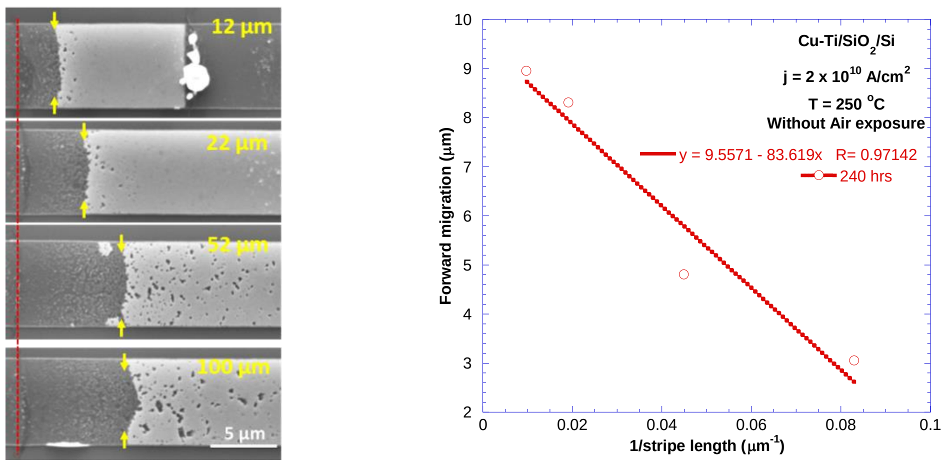
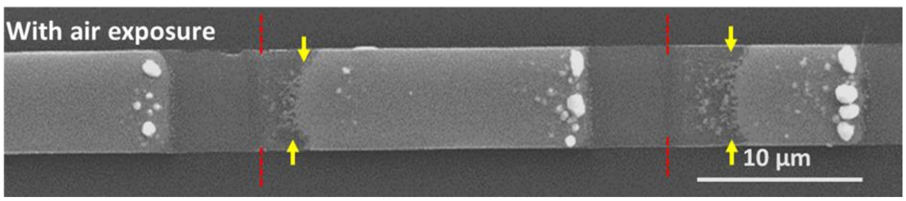


Figure 3: (a) SEM micrographs of Cu films in Cu-Ti system showing region near the cathode after 14,400 min (or 240 h) of electric current loading. The red broken vertical line shows the initial location of the Cu film, whereas the yellow vertical arrows in each stripe show the end of the Cu film after the test. (b) Variation of the forward migration or the extent of the depletion zone at the cathode as function of the inverse of the stripe length. The open symbols are the datum points, whereas the broken lines are the best fit curves. Equation for the best fit curve, along with the curve fitting parameters are shown in the legend.

Finally, the experiments performed by cycling the temperature of the Cu-Si samples between -50 to 150 ^{o}C revealed a significant role of the interlayer on the extent as well as the nature of plastic deformation in Cu (see **Figure 5)**. These experiments were performed by depositing Cu square islands on Si substrate with different interlayers (e.g., no interlayer, W and Ni) and by measuring the extent of sliding of Cu film (see **Figure 5d**). Herein also, *the samples with the strongest bond between Cu film and the interlayer showed the least amount of the* *sliding between Cu and Si, and hence the least change in the shape of Cu islands.* For example, more interfacial sliding was observed in the metallic-covalent bonding system (i.e., Cu on Si) than the metal-metal interface bonding (i.e., Cu with W/Ni interlayers). In addition to interfacial sliding, a few Cu grains also protruded to accommodate the CTE mismatch induced stresses after very larger number of cycles. Formation of hillocks ad their heights depend on the temperature range and heating rate.

(a)



(b)

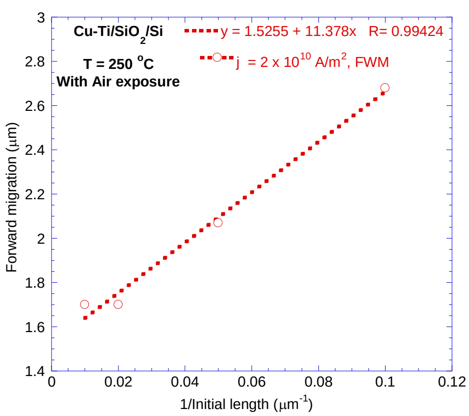
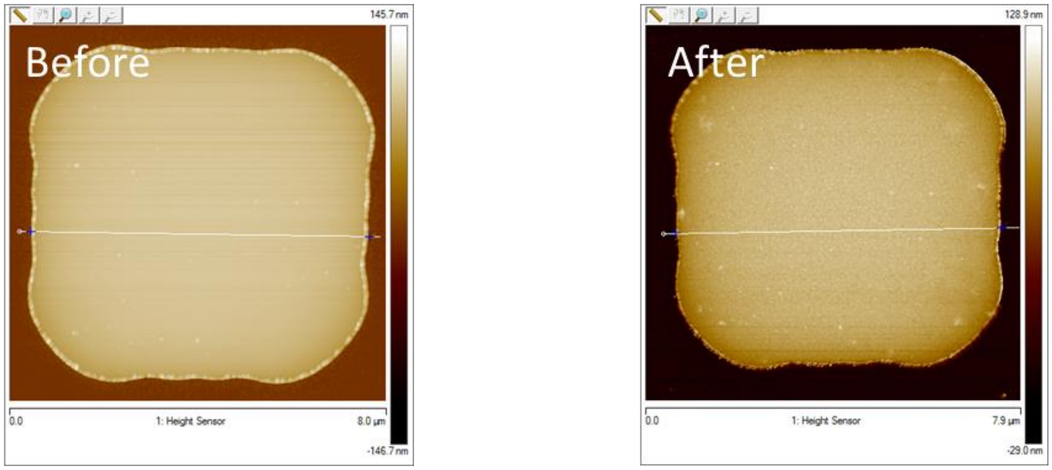


Figure 4: (a) Representative SEM micrograph showing Cu film in Cu-Ti-Si system (with Ti exposed to air for a few seconds prior to deposition of Cu) after passage of electric current of nominal density of 2×10^{10} A/m^2 at 250 °C for 1500 min. Red broken vertical line shows the initial location of the Cu film, whereas yellow vertical arrow shows the end of the Cu film after the test. (b) Variation of extent of the depletion zone at anode as function of inverse of the stripe length.

In summary, mass transport in Cu-Si system can be predicted by understanding the role of the sample geometry, coupling between various driving forces and the interlayer between Cu and Si. Such an understanding also provides a road map for the selection of new materials as interconnect as well as barrier/linear material that can be used in new microelectronic devices.

(a) (b)



(c) **(d)**

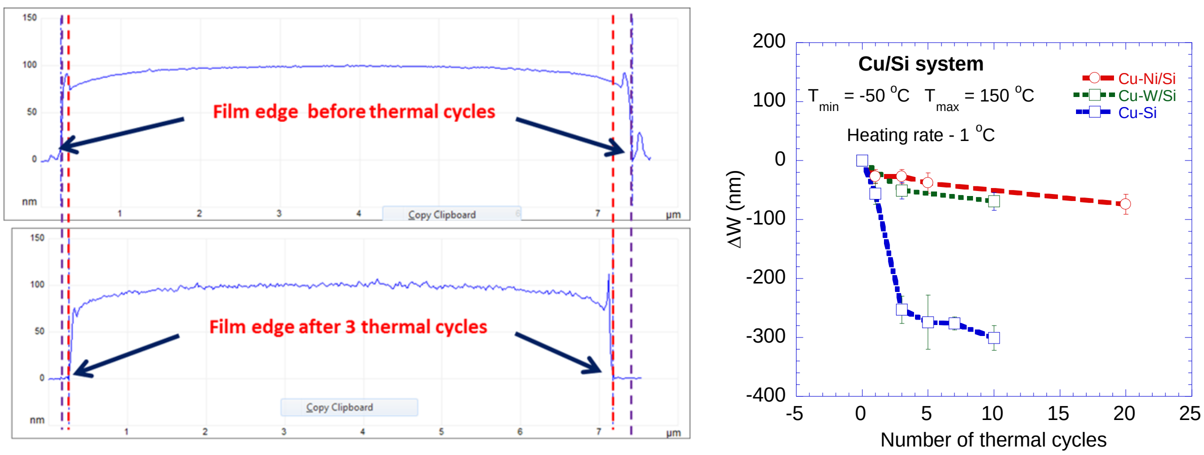


Figure 5: Topography of a Cu island deposited directly on Si (i.e., without an interlayer) as obtained using an AFM (a) before and (b) after 3 thermal cycles between -50 and 150 ºC. (c) Representative line scans along one of the medians before and after 3 thermal cycles. (d) Variation of the interfacial sliding, measured in terms of change in the width of Cu islands, as function of thermal cycling in Cu-Si system with various interlayers.