In situ TEM investigation of the deformation mechanism of thick copper metallizations

Liz Karanja[a*], Marc Legros[a],

[a] *CEMES-CNRS, 29 rue Jeanne Marvig 31055 Toulouse, France*

The structure of power semiconductor devices is constantly evolving to meet industry demands for higher power density, operating temperatures, miniaturisation and reliability. Typically, these devices contain several layers of different materials with different coefficients of thermal expansion (CTE) that induce thermomechanical strains and fatigue in operation. During fast switching between on and off states, the temperature in the device can rise to over 200°C and the associated differences in CTE produces high mechanical stresses that can cause irreversible deformation of the various layers, ultimately leading to device failure. In silicon-based devices, an example of this damage is the surface roughening and cracking of the thin top metal layer (usually aluminium (Al)).
The transition from Al to Copper (Cu) metallization is one of the major improvements in power semiconductors that has significantly increased the possible operating temperature, switching frequency and reliability of devices. Several modifications were implemented such as the deposition technique from sputtering to electrochemically deposited films (ECD). The Cu metallization thickness was also increased from 5µm to about 20µm to improve their reliability and provide the mechanical stability of thick Cu ultrasonic wire bondings connected to them.
To investigate the deformation of these thick Cu films , Moser et al [1] designed microelectronic chips that have been customized to replicate the heating rates and temperatures in real applications for 20µm Cu metallization deposited on Silicon wafers. Joule heating through an electrically resistive polysilicon layer generates the heating pulses; these devices are commonly referred to as polyheaters and serve as the devices under test for this work.

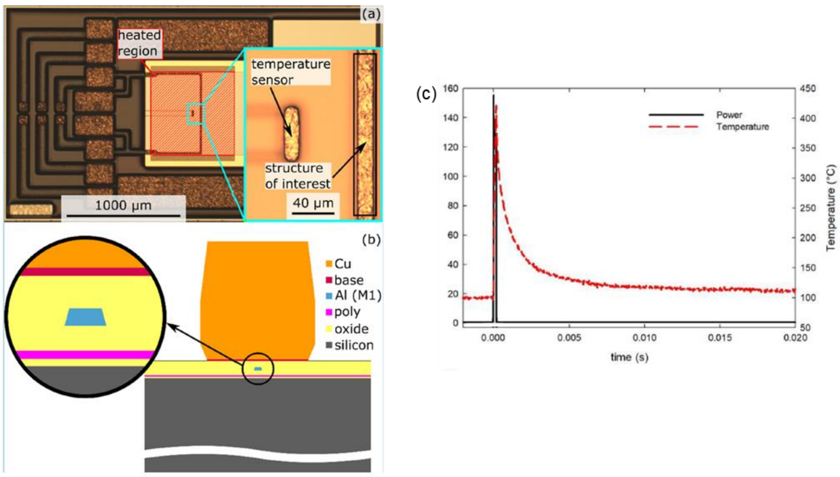

Figure 1 (a) An optical micrograph of the test chip used to thermal cycle rectangular Cu pad of 700×700×20µm^3 (b) Schematic representation of the cross-section showing the layers beneath the Cu metallization. The electrically resistive poly (polycrystalline silicon) layer facilitates the active heating of the chip via Joule heating (c) An example of the pulse with heating duration of 0.2ms applied to the Cu pad that results in temperature pulse of 100-400°C [1]

Moser et al [1] demonstrated that for base temperatures of ≥ 95°C the heating duration (length of pulses) dictates the degradation observed in the films. In this instance it is seen that shorter heating rates (0.2ms) result in inter granular cracking while for longer heating rates (5.4ms) the main degradation observed is extensive surface reconstruction. This work focuses on the microstructure evolution of the Cu films in which the heating duration is 0.2ms and the base temperatures of about ≥ 95°C. From the SEM surface images (Figure 1) we observe that as the number of cycles increases the apparition of pores is observed. The size and the occurrence of these pores increase as the cycles increase. After about 10k cycles we observe that the cracks have propagated from the surface of the film to the barrier in between the copper and silicon. A recent investigation on synchrotron dark field X-ray microscopy and in situ and ex situ scanning microscopy have attributed this degradation to the intragranular microstructural refinement and a gradual condensation of structural defects near high angle grain boundaries as driving forces for void formation in thick Cu films [2].

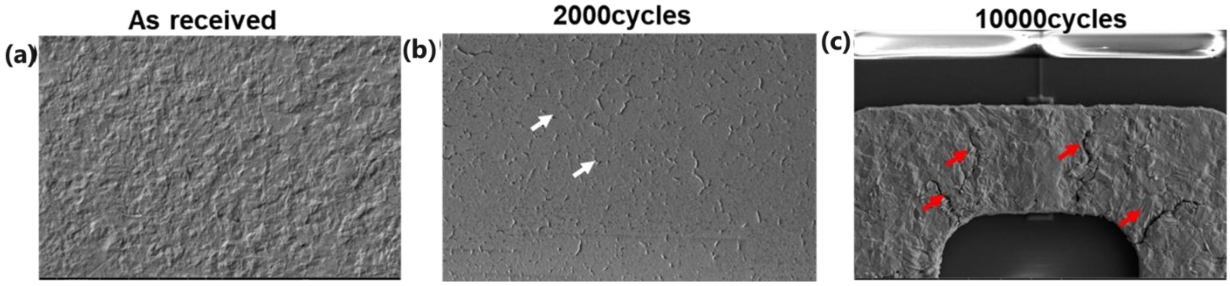

Figure 2 The evolution of the pore structure after several pulses. The white arrows point to the pores and the red arrows indicate the cracks on the surface of the thin film

In comparison to bulk materials, metallic films deposited on hard substrate deform in different manner with several intrinsic factors affecting their degradation such as their microstructure, grain size, film thickness… A common way to assess their mechanical properties and deformation mechanisms is to observe the thermal stress evolution during a heating and cooling sequence (also known as the wafer curvature experiment).

During a given thermal cycle, the biaxial stress in the film is measured through wafer curvature and the Stoney equation at heating rate on the order of 10°C/min [3]. This results in stress-temperature curves where the elastic to plastic deformation of these films can be monitored. These curves where subsequently interpreted to lay down hypothesis on the possible deformation mechanisms responsible for their degradation. Nonetheless, most of the hypothesis presented based on these curves such as the reversible motion of threading dislocations [4], the dislocation glide [5] and the combination of several mechanisms (dislocation glide, creep and grain boundary diffusion) [6] at different temperatures and stresses could not explain degradation features such as surface roughening and crack formation.

In-situ TEM (Transmission Electron Microscopy) has proven to be effective in directly observing the microstructural changes induced by the thermal cycling of thin films by partially reproducing thermal stresses acting on the metal part. Particularly in Al films the work of Martineau et al and Rufilli et al [7-8] have shown that the TEM is a direct way to confront existing deformation models, particularly those based on easily observable defects such as dislocations. As the dislocations are progressively trapped in grains, sub-grain boundaries and interfaces, a qualitative model based on grain-boundary accelerated diffusion was presented to explain the crack initiation and propagation during the thermal aging of Al films . Similar in-situ TEM observations where carried out in a previous study on thick copper films cycled at low base temperature (50°C) and longer heating durations (4.5sec)[9]. It corroborates the hypothesis that within the initial thermal cycles, the intragranular microstructural refinement is mainly caused by dislocations gradually reorganizing themselves into cell structures.

As the cycling rates increase the behaviour of dislocations (intragranular structure) may change, and so their, contribution to the voiding and fracture observed in the films. This work aims to utilize advanced microscopy techniques such as conventional and in-situ TEM to elucidate the mechanisms responsible for pore formation and crack propagation in thick Cu films.

References

[1] S. Moser, M. Kleinbichler, J. Zechner, M. Reisinger, M. Nelhiebel, and M. J. Cordill, Fatigue of copper films subjected to high-strain rate thermo-mechanical pulsing, Microelectronics Reliability **137**, 114782 (2022).

[2] K. Hlushko, T. Ziegelwanger, M. Reisinger, J. Todt, M. Meindlhumer, S. Beuer, M. Rommel, I. Greving, S. Flenner, and J. Kopeček, Intragranular thermal fatigue of Cu thin films: Near-grain boundary hardening, strain localization and voiding, Acta Materialia **253**, 118961 (2023).

[3] S. Bigl, C. O. W. Trost, S. Wurster, M. J. Cordill, and D. Kiener, Film thickness dependent microstructural changes of thick copper metallizations upon thermal fatigue, J. Mater. Res. **32**, 2022 (2017).

[4] W. D. Nix, Mechanical properties of thin films, Metall Trans A **20**, 2217 (1989).

[5] P. A. Flinn, D. S. Gardner, and W. D. Nix, Measurement and Interpretation of stress in aluminum-based metallization as a function of thermal history, IEEE Trans. Electron Devices **34**, 689 (1987).

[6] M. Thouless, J. Gupta, and J. Harper, Stress development and relaxation in copper films during thermal cycling, Journal of Materials Research **8**, 1845 (1993)

[7] Martineau, D., Levade, C., Legros, M., Dupuy, P., & Mazeaud, T. (2014). Universal mechanisms of Al metallization ageing in power MOSFET devices. Microelectronics Reliability, **54**(11), 2432-2439

[8] Ruffilli, R. (2017). *Modes de fatigue des métallisations à base d'aluminium dans les composants MOSFET de puissance| Theses. fr* (Doctoral dissertation, Toulouse 3)

[9] Karanja, L. (2024) Mécanismes d'endommagement des interconnexions en cuivre et en aluminium dans les IGBT de puissance. *Theses. fr* (Doctoral dissertation, Toulouse 3).