Cu Pumping Analysis during Cu/SiO_2 Hybrid Bonding using In-situ SPM Imaging

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***Abstract*— The assessment of Cu pumping (also known as Cu extrusion) during thermal annealing is vital information for the successful execution of hybrid bonding as well as defect-free processing of the through silicon vias (TSV). Unpredicted Cu pumping can pose major reliability issues. Correspondingly, in this study, high-temperature analysis of Cu pumping was conducted utilizing in-situ scanning probe microscopic (SPM) imaging. Cu / SiO_2 surfaces with recessed and protruded Cu topographies were produced by chemical mechanical polishing (CMP) and used for Cu pumping investigations. The amount of Cu pumping upon thermal annealing up to 400 °C and cooling down to room temperature was precisely quantified. The SPM results were compared with FEM simulation results, and a numerical equation for Cu pumping was proposed, accordingly. It was shown that by using in-Situ SMP imaging, valuable information on the behavior of hybrid Cu / dielectric surfaces can be generated.**

Keywords—Cu pumping, SPM, Nanoindentation, Hybrid bonding, Cu Extrusion, TSV, BEOL, CMP

I. INTRODUCTION

Hybrid bonding and Through Silicon Via (TSV) technologies are the two key processes for 3D integration enabling "more than Moore" scaling. Hybrid bonding has recently emerged as the preferred direct wafer-level bonding approach for creating high-density interconnects. TSVs are also widely utilized for both 2.5 D interposer-type integration as well as 3D IC stacking. Hybrid bonding consists of dielectric surface activated bonding (SAB) at low temperatures followed by thermal annealing up to 400 °C to facilitate copper (Cu) bonding. For a successful hybrid bonding, the chemical-mechanical polishing (CMP) processing of the Cu/ dielectric plays a critical role where the surface roughness, uniformity and dishing depth can be influenced. Moreover, the annealing process parameters can highly impact the Cu-Cu bonding yield [1-5].

Hybrid bonding is usually executed using two wafers with recessed Cu surfaces (with dishing heights ranging from 5 to 10 nm) surrounded by a dielectric layer. The dielectric layer can be SiO_2, SiN, or SiCN. Recently, the employment of recessed Cu on one wafer and protruded Cu on the other wafer has received attention. This is owing to the creation of huge tensile stress after cooling in recessed-recessed bonds degrading the yield and long-term reliability of the bonds. The protruded-recessed bond can facilitate an optimized bondline shape for hybrid bonding [3]. The advantage of protruded-recessed Cu bonds for further downscaling of hybrid bonds to sub-µm dimensions was also reported before [4]. The relatively limited Cu expansion at sub-µm dimensions might be a concern for typical recessed-recessed hybrid bonding. The smaller gap size of protruded-recessed Cu bonds might be advantageous to avoid excessive annealing temperatures [4].

The assessment and control of Cu pumping during annealing is necessary for the successful execution of hybrid bonding as well as the processing of the through silicon vias (TSV) [6]. Cu pumping, which stems from Cu expansion due to differential CTE between Cu and the surrounding dielectric, is a stress release mechanism at high temperatures. The dominant mechanism for Cu pumping is diffusional creep [6, 7]. In fact, the coefficient of thermal expansion (CTE) of Cu is much higher (16.7 ppm/C) than the one of Si (2.3 ppm/C) and typical dielectric materials such as SiO_2/ SiN and SiCN. Consequently, Cu, which is confined within the dielectric or Si, will undergo compressive stress during any high-temperature processing. The weakest boundary where this stress can be released is the open surface on top of the via in hybrid bonding or the thin back end of line (BEOL) pad in TSV. Consequently, Cu extrusion in the vertical direction can be observed during any pre- or post-CMP annealing of TSVs, as well as heating associated with dielectric-deposition during the fabrication of BEOL or redistribution layer (RDL). Cu pumping increases with increasing temperature leading to the deformation and damage to the BEOL layers above in TSVs. Due to the plastic deformation of Cu, this effect cannot be completely reversed upon cooling to ambient temperature and only a very small elastic portion can be retracted [6].

Cu pumping had previously been studied using room-temperature metrology tools before and after thermal annealing using scanning white light interferometry (WLI) and atomic force microscopy (AFM). However, due to Cu's rapid oxidation at elevated temperatures, in-situ analysis of Cu pumping was not comprehensively investigated [4-8]. Usually, the amount of Cu pumping at high temperatures was estimated from simulation data. Additionally, both AFM and WLI have limitations when used as an in-line wafer-level process-controlling tool. For example, AFM is a relatively slow technique with a restricted scanning area, which does not easily allow for obtaining statistical information [6]. WLI, on the other hand, is a quick, contact-free, wafer-level technique. However, WLI is sensitive to surface optical properties, which is an issue for hybrid (Cu/dielectric) surfaces with different amounts of light reflection. In particular, for transparent layers such as SiO_2, WLI analysis can be challenging, as the optical properties and thickness of the SiO_2 layer should be known. Another approach is the deposition of a thin metal layer (e. g. 30 nm PVD Ta) on top of the sample [6].

In this study, an alternative methodology for in-situ analysis of Cu pumping based on scanning probe microscopy using nanoindentation imaging is introduced and investigated.

II. EXPERIMENTAL

In this study, 300 mm silicon test wafers with a Cu pad diameter of 4 µm and a pitch size of 10 µm surrounded by SiO_2 were used, as shown in Fig. 1. The area fraction of Cu at the surface of the chips was 12,5%. By using two different CMP recipes, wafers with Cu protrusion of + 13 nm and wafers with Cu recession of -9 nm relative to SiO_2 surface were generated. The effects of CMP processing parameters (e.g. Cu/ barrier polishing slurries, pads, polishing pressure, duration, and polishing rate selectivity) on the topography of Cu were described in [9].

In-situ scanning probe microscopy (SPM) was carried out using a Hysitron TI Premier nanoindenter (Bruker Corporation, USA). SPM is a contact-mode profilometry technique that employs a piezo scanner to sweep the indenter tip across the sample surface, monitoring any changes caused by topography or surface roughness [10]. A Berkovich indenter was used to perform in-situ SPM imaging. An extremely low contact force of 2 µN and a scan rate of 1 Hz was applied during raster scanning of the samples, while an area of 25 × 25 µm was analyzed in different temperatures. Both recessed and protruded Cu wafers were examined.

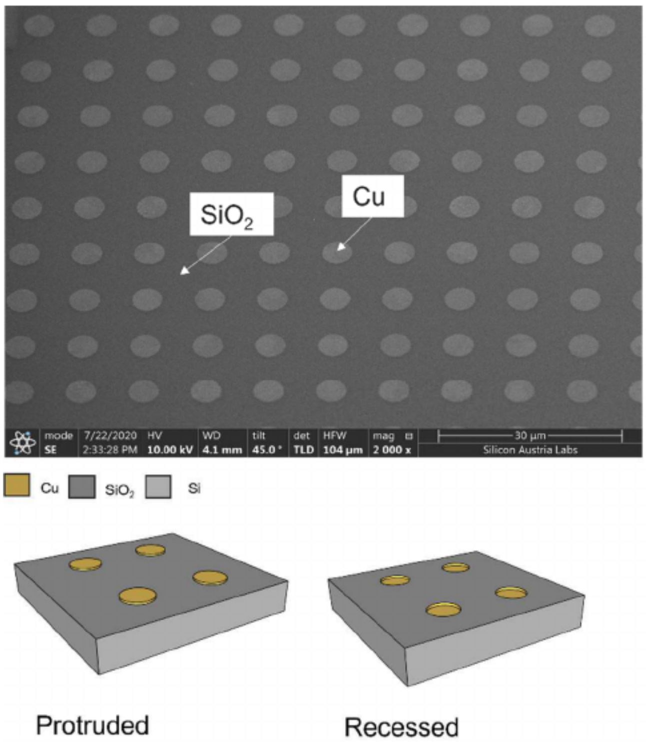

Fig. 1. An SEM image of the sample used in this study with a Cu pad diameter of 4 µm (top) and schematic demonstrations of the generated protruded and recessed topographies after CMP processing (bottom).

The samples were placed in a heating stage with resistive heating elements and kept in an N_2 environment during the measurements. SPM was performed up to 400 °C, while the temperature of the sample was controlled using a precisely calibrated PID feedback loop. Each SPM mapping took less than a minute. Also, the heating time to 400°C was less than a minute. The high-temperature SPM imaging setup and the temperature analysis of the setup indicating the uniform temperature distribution over the sample are shown in Fig. 2.

In addition to the experiments, Cu pumping was also simulated using the finite element method (FEM) in ANSYS 21.2. Both simulation results and SPM measurements were compared and used to define a formula for Cu pumping which will be discussed later.

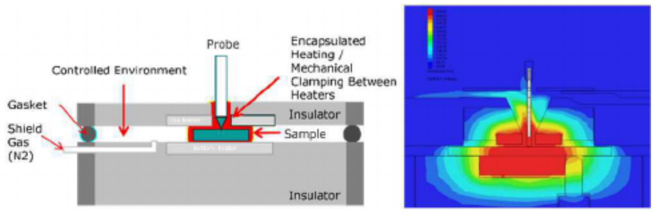

Fig. 2. High-temperature SPM imaging setup (left) and the temperature analysis of the setup indicating the uniform temperature distribution over the sample (right)

III. RESULTS

Fig. 3 depicts the 3D topographical maps of the recessed and protruded samples before, during, and after 400 °C annealing. An area of 25 × 25 µm consisting of 8 Cu pads was selected for these investigations.

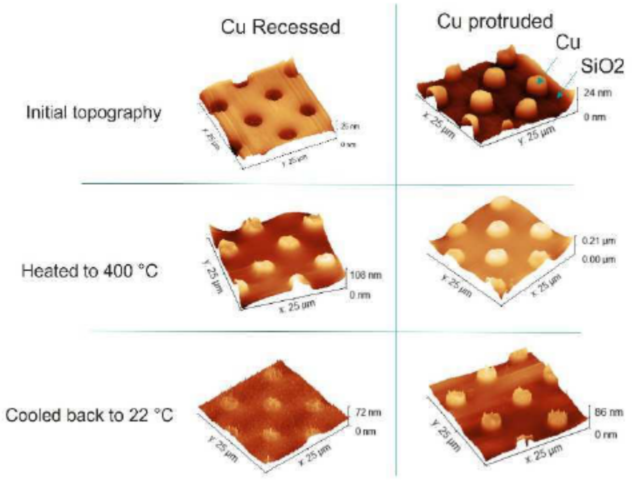

Fig. 3. SPM mapping results of two types of Cu/SiO_2 topographies (recessed and protruded) before annealing, heated to 400 °C and after cooled back to room temperature

Correspondingly, the section profiles of the samples are plotted in Fig. 4. As shown here, Cu in the recessed samples expands to 40 nm at 400 °C and retains 9 nm above the SiO_2 surface after cooling. Similarly, in protruded samples, the Cu pumping reaches 65 nm at 400 °C and remains 28 nm above the surface after cooling to ambient temperature. It can be inferred from these results that Cu pumping is an irreversible extrusion of Cu due to the occurrence of plastic deformation upon annealing which relaxed the high compressive stress in Cu [11].

The FEM simulation results of Cu pumping are also shown in Fig. 5. All materials are considered linear isotropic. Temperature variations in Young's modulus of Cu, as well as the coefficients of thermal expansion of SiO_2, Cu, Si and Ti, were also taken into consideration. The nonlinear stress-strain relationship of the Cu was implemented in the simulation by using the Ramberg-Osgood model [12, 13].

pads It can be estimated that the maximum amount of Cu pumping ($h_{max@\ 400\ °C}$) was around 51 ± 3 nm for both recessed and protruded Cu.

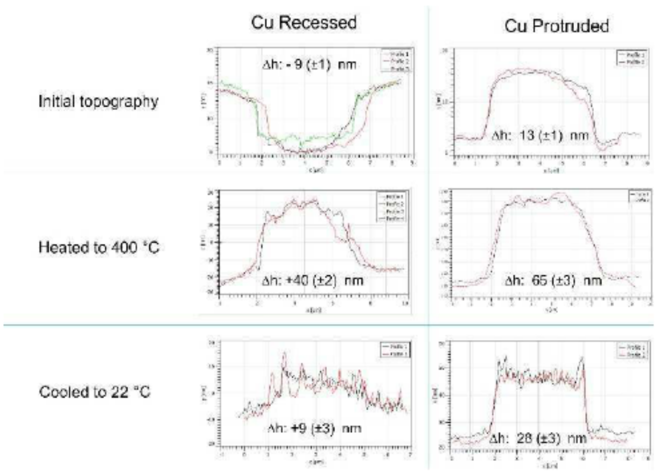

Fig. 4. SPM profilometric analysis of the samples upon thermal annealing

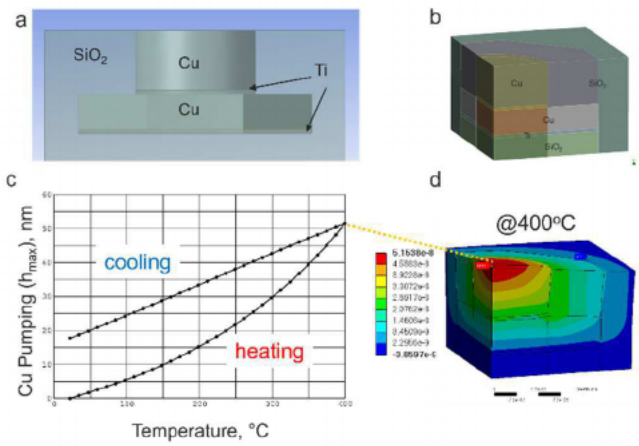

Fig. 5. FEM simulation results of Cu pumping upon heating to 400 °C. (a) and (b) illustrate the model geometry, (c) shows a gradual increase of Cu deformation upon heating to 400 °C and cooling back to room temperature. (d) presents the region with the maximum Cu deflection (h_{max})

TABLE I THE SUMMARY OF SPM AND SIMULATION REUSLTS

Recessed Cu	Condition	Simulation Δh [nm]	Experiment Δh [nm]
	@ 22 °C (initial)	-9.00	-9 ±1
	@ 400 °C	42.3	40 ±3
	@ 22 °C (after cooling)	8.6	+9 ±3
Protruded Cu	**Temperature [°C]**	**Simulation Δh [nm]**	**Experiment Δh [nm]**
	@ 22 °C (initial)	13	13 ±1
	@ 400 °C	64.5	65 ±3
	@ 22 °C (after cooling)	30.1	28 ±4

Table 1 summarizes the SPM experimental and FEM simulation results, implying a good agreement between them. Here Δ*h* was defined as the average height difference of Cu in the middle of the pad to the SiO_2. As mentioned before, the reported measurement values are the average of those for 8 Cu pads It can be estimated that the maximum amount of Cu pumping ($h_{max@\ 400\ °C}$) was around 51 ± 3 nm for both recessed and protruded Cu.

IV. DISCUSSION

As demonstrated in the previous section, utilizing in-situ metrology can be a valuable asset for providing reliable simulation input parameters and validating simulation output. Employing the empirical data obtained from SPM profilometric results and a feedback loop to the FEM model can provide a deeper understanding of the underlying mechanical behavior and expansion mechanisms of Cu. Given that, an attempt has been made to derive numerical equations for the maximal Cu pumping (h_{max}) at the annealing temperature as a function of Young's moduli and coefficient of thermal expansion (CTE) of Cu and dielectric materials. For this purpose, other dielectric materials such as SiN and SiCN were also fabricated and examined. For instance, the maximum amount of Cu pumping at 300 °C ($h_{max@300\ °C}$) can be expressed as a function of Young's moduli of Cu (E_{Cu}) and the dielectric material (E_d) as well as the CTE of the dielectric (α_d) as follows:

$$h_{max\,@\,300°C} = A(\alpha_d) + B(\alpha_d) * ln\,(E_d/E_{Cu}), \qquad (1)$$

where

$$A(\alpha_d) = 40.415 + 1.3771 * 10^6 * \alpha_d \qquad (2)$$

and

$$B(\alpha_d) = 8.3373 + 1.3177 * 10^5 * \alpha_d\ . \qquad (3)$$

As inferred from Eq. 1, the amount of Cu pumping has a logarithmic relationship to E_d/E_{Cu}. This means that a hybrid surface consisting of Cu with the highest stiffness and dielectric with the lowest stiffness can yield the minimum amount of Cu pumping. In other words, the greater the stiffness of the dielectric, the greater the Cu pumping; since the expansion of Cu in the radial direction is more constrained.

The proposed formula holds great potential in optimizing both TSV processing and hybrid bonding in terms of Cu pumping prediction, ensuring reliable performance in various applications. Future work is currently underway to extend this equation including additional parameters such as temperature dependency, Poisson's ratio, and Cu microstructure, etc. In fact, Cu microstructure such as crystal orientation, and grain size can influence the amount of Cu pumping. In a previous study, a correlation between Cu pumping and Cu microstructure based on the grain size at the top of TSV was reported, where the TSVs with a higher number of grains showed a higher amount of Cu pumping. This was attributed to the fact that high-angle grain boundaries enhance both diffusion creep rate and dislocation creep rate, rendering higher Cu pumping [11].

V. CONCLUSION

In this study, Cu pumping in hybrid Cu/ SiO_2 surfaces was analyzed and quantified using in-situ SPM imaging at different temperatures. The maximum amount of Cu pumping was found to be 51 ± 3 nm for both recessed and protruded Cu topographies. The irreversible deformation of Cu after cooling back to room temperature was also verified. The experimental results showed good agreement with the FEM simulation results. By implementing both empirical data from SPM and the results of a parametric simulation study, Cu pumping at high temperatures was consequently presented as a numerical function of Young's moduli and coefficient of thermal expansion (CTE). The proposed equation (Eq.1) provides a deeper understanding of Cu pumping and the underlying material parameters, laying a solid foundation for future investigations.

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