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Application of a Metallic Cap Layer to Control Cu TSV Extrusion

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Abstract --In this study, we report the reduction of via extrusion for Cu through-silicon vias (TSVs) through the application of a metallic cap layer. The basic idea of this approach is based on suppressing the mass transport which causes via extrusion on the top surface of TSVs. Two materials, W and Co, were deposited as the cap materials. Experiments were carried out to characterize the extrusion behavior and shown that both materials were able to reduce the average and maximum extrusion height in the TSV sample comparing to a reference TSV sample without the cap layer. In addition, the results suggest that Co is more effective than W to suppress via extrusion, as Co is known to be a good diffusion barrier, while W is immiscible with Cu. The underlying mechanism for the cap layer effect is discussed.

Keywords-3D Integration; TSV; Extrusion; Plasticity; Stress; Interface

I. INTRODUCTION

Through-silicon vias (TSVs) is a key enabling element for three-dimensional (3D) integration, which delivers distinct advantages in integration density, device performance, form factor and power efficiency [1-3]. In the commonly-used via-middle approach, TSVs are fabricated after completion of front-end-of-the-line (FEOL) process and prior to back-end-of-the-line (BEOL) process, and key steps of via fabrication involve deep etching of via holes, deposition of an oxide layer on the sidewall, deposition of barrier and seed layers, electroplating of Cu, and chemical-mechanical planarization (CMP) removal of the Cu overburden. Despite the advantages they bring, TSVs carry their own concerns as a result of the manufacturing and working process. The via middle process exposes the Cu TSVs to multiple thermal cycles, which will lead to considerable thermal stresses in and around the TSVs since the difference in the coefficient of thermal expansion (CTE) between Cu (α_{Cu}=17ppm/°C) and Si (α_{Si}=2.3ppm/°C) is very large. The resulted thermo-mechanical issues raise reliability concerns during the fabrication, testing and operation of TSV structures. Among the thermal stress-induced reliability issues of TSVs, via extrusion, which is the non-recoverable plastic deformation near the top of the via after thermal processing, is particularly important, as the protrusion of Cu vias in the axial direction can deform and crack BEOL interconnect layers to fail the device [4].

Different approaches have been proposed to control via extrusion, such as adding a post-plating annealing process and reducing via diameters [5-7]. Although these methods have been shown to reduce the average values of via extrusion, recent studies reveal that the height of via extrusion exhibits a statistical variation. The statistical variation of via extrusion height is important, as the actual BEOL reliability will be determined by the weakest link, i.e., the 0.1% of TSVs with the highest extrusion heights. The stochastic nature in via extrusion may be traced to the stochastic nature of grain structures near the top of the vias, although the effect is not fully understood. It is also not clear how existing approaches can be effective in containing the tail portion of the extrusion height distribution [7-9]. Both reducing the via extrusion and improving the statistics of its distribution are important, as the overall reliability of a 3DIC containing many TSVs will be limited by a small percentage of TSVs with largest extrusions.

In this study, we report an approach which can effectively reduce via extrusion and potentially improve its statistics by the application of a metallic cap layer. The idea is to suppress the Cu diffusion path at the via top, which directly contributes to mass transport causing via extrusion. We successfully demonstrate considerable reduction of via extrusion and discuss how the statistical variation can potentially be controlled by the applied metallic cap layer.

II. EXPERIMENTS

A. Test vehicle

The TSV samples used in this study were blind Cu TVSs in a 780 µm thick (001) Si wafer fabricated using standard etching and electroplating processes. The dimension of the TSV is 5.5 µm ×50 µm (diameter × height) and the thickness of the oxide liner at the via side wall was about 0.4µm. No post-annealing was carried out after via filling.

In this study, both W and Co were used as the metallic cap layer and their deposition was carried out using a sputtering system. Prior to coating the cap layer, TSV samples were treated to remove the natural Cu oxide formed at the via top by dipping in acetic acid and followed by ultrasonic cleaning

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with Acetone, IPA and DI water. The thickness of the cap layer was determined by a quartz crystal thickness monitor and confirmed by atomic force microscopy (AFM). For both W and Co, the cap layer thickness was 50nm. The sample with the cap layer will be referred to as “capped sample”, and the same TSV structure without the cap layer will be referred to as “reference sample”. A TSV sample with a cap layer covering its top surface is illustrated in Fig. 1.

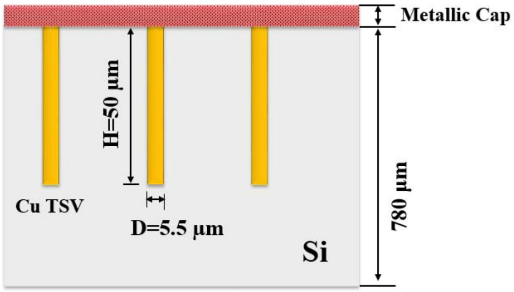


Figure 1. Illustration of the blind via test structure with cap layer. The dimension of the TSV is 5.5µm×50µm (diameter × height), the thickness of the Co cap layer is 16nm, and the Si wafer is 780 µm.

B. Via extrusion measurement

To study the via extrusion behavior, both W and Co capped samples and a reference sample were annealed at 400˚C for 1 hour in a forming gas atmosphere (Ar-4%H_2) with the heating rate of 6°C/min. After annealing, AFM scans were carried out to obtain the surface profiles of the vias. For both the reference sample and the W capped sample, 95 vias were measured. For the Co capped sample, 20 vias were measured. From the scan data, the maximum via height h_{max} and the average via height, h_{avg}, were obtained. The height of the vias before annealing was also measured by AFM and was determined to be $h_0 = 5.6\,nm$. The maximum extrusion of a TSV was then determined as $\Delta_{max} = h_{max} - h_0$, and the average extrusion was $\Delta_{avg} = h_{avg} - h_0$.

C. Substrate curvature measurement

In addition to extrusion height measurement, substrate curvature measurements were performed on both a reference sample and a sample with Co cap layer to study the effect of the cap layer on the thermo-mechanical behavior of the vias. The curvature is measured based on an optical lever setup with two position-sensitive photodetectors tracking the movement of the reflected laser spots due to sample bending during thermal cycling tests [10]. To simulate the annealing condition, both samples were heated at 6°C/min to 400°C and held at 400°C for 1 hour, before cooling down to RT. After the test, Cu was etched away and the same samples now without Cu were measured again under the same temperature-time profile to obtain a reference curvature, κ_0. After subtracting κ_0, the net curvature changes, $\Delta\kappa$ can be obtained. Detailed description of the substrate curvature technique can be found in reference 10.

III. RESULTS

A. Via extrusion

The cumulative distribution function (CDF) of the average extrusion, Δ_{avg} and maximum extrusion, Δ_{max} were plotted in Fig. 2 for the 95 vias measured in the reference sample. The CDF of Δ_{avg} and Δ_{max} for the 95 vias measured in the W coated sample was plotted in Fig. 3. For Co capped vias, the height profile of only 20 vias were obtained and the results were shown in Fig. 4.

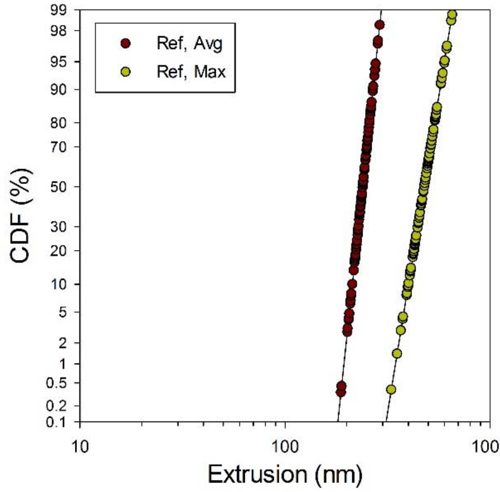


Figure 2. Cumulative distribution function (CDF) plots of average via extrusion and maximum via extrusion for 95 vias in the reference sample.

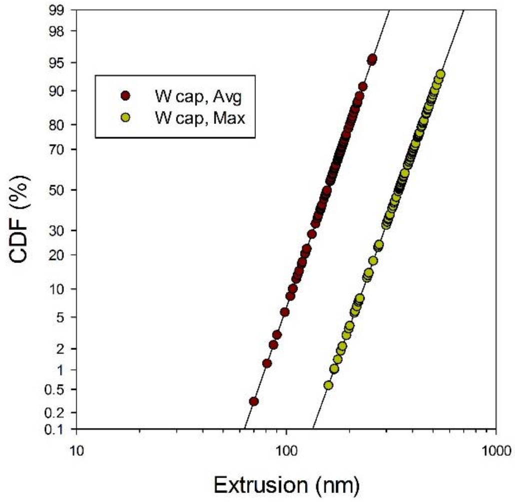


Figure 3. Cumulative distribution function (CDF) plots of average via extrusion and maximum via extrusion for 95 vias in the W capped sample.

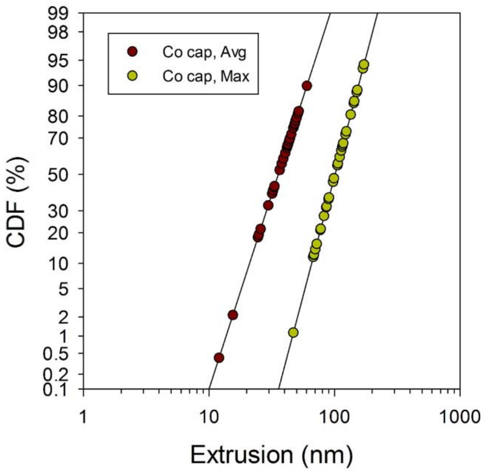
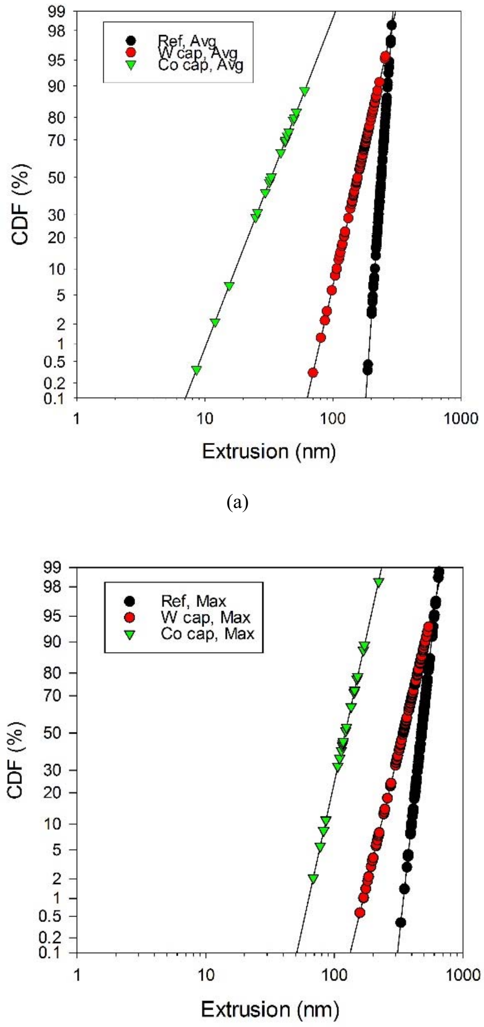


Figure 4. Cumulative distribution function (CDF) plots of average via extrusion and maximum via extrusion for 20 vias in the Co capped sample.

In all three cases, both the average and maximum via extrusion heights can be described by the lognormal distribution. The statistical nature of via extrusion is quite obvious from the wide spread of the extrusion height. For example, Δ_{avg} of the 95 reference vias ranges from 187nm to 290 nm, with an average of 240 nm. Δ_{max} for the reference vias ranges from 329 nm to 660nm, with the average of 482nm. This kind of statistical via extrusion behavior is consistent with previous observations and may be traced to the stochastic nature of Cu grain structure near the top of the via [8,9,11]. In particular, grain boundary diffusion may play a major role in causing the statistical variation of the via extrusion [9].

Comparing to the reference sample, which does not have the metallic coating on the top surface of the vias, the W capped and the Co capped samples showed considerable reduction in both Δ_{avg} and Δ_{max}. For example, Δ_{avg} of the 95 W capped vias ranges from 45 nm to 258nm, with an average of 163 nm. Δ_{max} for the W capped vias ranges from 158 nm to 543 nm, with the average of 359 nm. Comparing to the reference sample, the W capped vias showed about ~32% and 25% reduction in Δ_{avg} and Δ_{max}. The reduction of via extrusion can be seen in the CDF plots in Fig. 5, where Δ_{avg} and Δ_{max} for the reference sample, as well as the W and Co coated samples were plotted. The plots also show that despite the smaller via population used to plot the Co capped vias, Co seems to be a more effective cap material than W in reducing via extrusion.

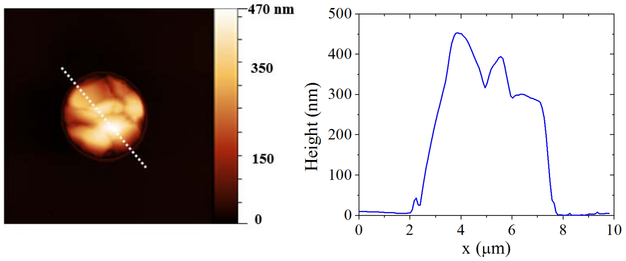


(a)

(b)

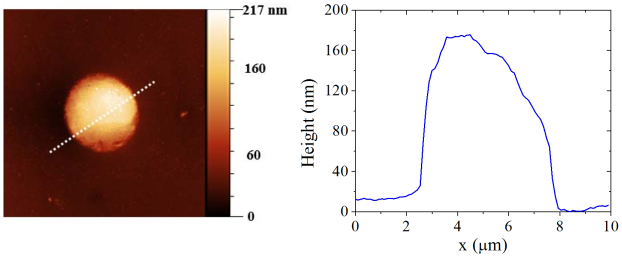
Figure 5. Cumulative distribution function (CDF) plots for the reference vias, vias with 50nm W cap, and vias with 50nm Co cap. (a) Average via extrusion. (b) maximum via extrusion

This reduction in via extrusion is also obvious from the AFM scans. In Figs. 6-8, a representative AFM image is shown for a reference via without the cap layer, a via with 50nm W cap layer, and a via with 50nm Co cap layer. The height profile along the via top was also extracted and plotted for each case. In addition to the reduced via height, the AFM results show that with the presence of a cap layer, the roughness at the via top was much reduced. This can be seen by comparing the granular appearance in the reference vias to the smoother, dome-shaped profiles for the vias with the thin cap layers.



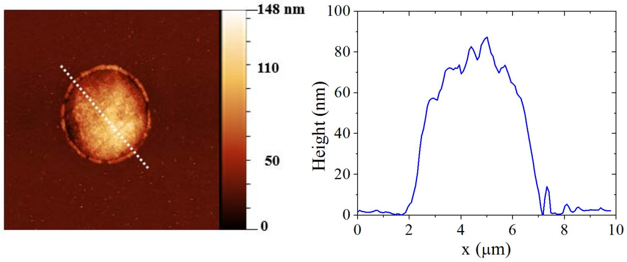
(a) (b)

Figure 6. AFM scan of a reference via. (a) height contour at via top surface; (b) heigh profile along the dashed line across the via top.



(a) (b)

Figure 7. AFM scan of a W capped via. (a) height contour at via top surface; (b) heigh profile along the dashed line across the via top.



(a) (b)

Figure 8. AFM scan of a Co capped via. (a) height contour at via top surface; (b) heigh profile along the dashed line across the via top.

B. Stress relaxation

For the reference TSV sample and the sample with Co cap, the curvature changes during the 1 hour isothermal relaxation segment at 400ºC were plotted in Fig. 9. For an easier comparison of the relaxation magnitude, the curvature at t=0, which is the beginning of the isothermal test, was shifted to the same point, which will not affect the qualitative comparison of the curvature behaviors between these two samples. Comparing to the reference sample, the sample with Co cap layer shows slower rate of curvature change. This is an indication that the rate of stress relaxation is much reduced, and will be discussed further in section IV.

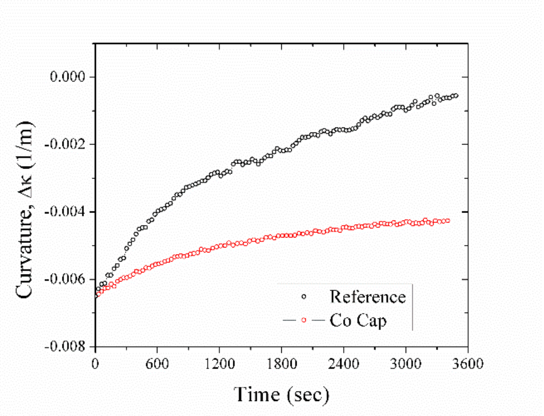


Figure 9. Curvature change during isothermal annealing of the reference sample and sample with Co cap layer at 400ºC for 1 hour.

IV. DISCUSSION

A. The effectiveness of a cap layer in reducing via extrusion

The results shown that via extrusion was reduced when a thin metallic cap layer was applied at the top of the TSVs, and that the degree of reduction is different with the choice of cap material. When Co was used as the cap material, a much larger degree of reduction was achieved. This may be explained by looking at the mechanisms causing via extrusion, especially by considering the mass transport process contributing to via extrusion.

For Cu thin film deposited on a substrate, it has been shown that when a passivation film is deposited on the surface of the film, diffusional creep can be reduced by inhibiting the source of migrating atoms or vacancies [12-15]. Similarly, the effect of a cap layer in improving via extrusion reliability can be understood by considering the mass transport process contributing to via extrusion.

Diffusional creep along the grain boundaries and/or the via/liner interface is an important mechanism causing via extrusion at the TSV processing temperature, along with other mechanisms such grain growth and plastic yielding by dislocation glide [16]. At the grain boundaries and the via/liner interface, the disordered atomic arrangements provide paths for fast diffusion. When the TSVs are subjected to thermal cycling, stress-driven diffusion along grain boundaries and/or the via/liner interface leads to accumulation of Cu atoms on the via surface, which manifests as via extrusion. This process is illustrated in Fig. 10a. When a cap layer is present, similar to the case for passivated Cu thin film, the source of migrating atoms or vacancies may be much limited, therefore reducing the driving for mass transport and reducing via extrusion. This situation is illustrated in Fig. 10b. This also explains the reduction of surface roughness observed for the capped vias, since the mass transport along grain boundaries contribute to the uneven extrusion profile. Additionally, the curvature relaxation measurement shown in Fig. 9 further supports the mechanism shown in Fig. 10. Although qualitatively, it was clear that the presence of a Co layer reduced the rate of stress relaxation by reducing the mass transport responsible for stress relaxation, which is similar to the observation for passivated Cu thin film [14].

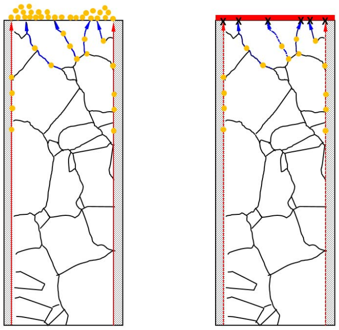


Figure 10. Isothermal annealing of the reference sample and sample with 16nm Co cap layer at 400ºC for 1 hour.

B. Choice of cap materials

In addition to suppressing mass transport by diffusion, mechanical constraint by the metallic cap is another possible mechanism to reduce the extrusion height. Past studies have shown that as a result of geometrical confinement by the surrounding Si, large stress concentration occurs near the top of the TSV, especially near the via/liner interface [17]. The presence of a cap layer on the via surface will alter the stress state by adding additional confinement in the vertical direction, and therefore can reduce the stress gradient driving plastic deformation. This is most likely what happened for the case of W capped TSVs, since W is immiscible with Cu and has high strength and modulus [18]. On the other hand, it has been shown that when Co is deposited on Cu, the Co/Cu interface can be highly coherent with minimal lattice disruption [19]. This is one of the reasons why Co is a very effective EM diffusion barrier for Cu interconnects and in the present study, could explain why Co is a very effective cap layer to reduce via extrusion. Similarly, the effectiveness of the cap layer on reducing via extrusion will be largely influenced by the interface structure between the cap and the top surface of Cu vias. Alternative cap materials which may react with the Cu underneath forming an alloying layer or partially dissolve into the Cu grain boundaries may be potential choices to effectively reduce via extrusion, as these material could have similar effect in reducing the mass transport causing extrusion.

C. Controlling extrusion statistics

As shown in this study and other work [7-9], the distribution of via extrusion has a wide spread, with the tail distribution at 99.9% of the distribution several times larger than the median extrusion value at 50% of the distribution. This is highly undesirable and can be traced to the stochastic nature of grain distribution in the TSVs near the top of the via, although the detailed mechanism need to be further investigated. Since the via population used in plotting Fig. 5 is relatively small, the effect of the cap layer on the statistics of via extrusion is still to be investigated. However, the fact that the surface roughness is much reduced based on the AFM scans, and the evidence that the cap layer can suppress mass transport along grain boundaries, make this approach promising for controlling the spread of via extrusion. Further studies are underway, and initial evidence suggest that indeed by optimizing the cap materials and the interface, the statistical spread of via extrusion can be improved.

V. SUMMARY AND FUTURE WORK

In summary, we demonstrated that a thin metallic cap layer can effectively reduce via extrusion and has the potential to improve the extrusion statistics. The mechanism of the cap layer in reducing via extrusion is attributed to the reduction of mass transport along the grain boundaries and interfaces by limiting the atom and vacancy sources at the via surface. The deposition of a cap layer is compatible with current TSV processing. With further studies, it would be possible to optimize the cap material to further improve via extrusion reliability.

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