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Plasticity mechanism for copper extrusion in through-silicon vias for three-dimensional interconnects

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In this paper, we demonstrated the plasticity mechanism for copper (Cu) extrusion in through-silicon via structures under thermal cycling. The local plasticity was directly observed by synchrotron x-ray micro-diffraction near the top of the via with the amount increasing with the peak temperature. The Cu extrusion was confirmed by Atomic Force Microscopy (AFM) measurements and found to be consistent with the observed Cu plasticity behavior. A simple analytical model elucidated the role of plasticity during thermal cycling, and finite element analyses were carried out to confirm the plasticity mechanism as well as the effect of the via/Si interface. The model predictions were able to account for the via extrusions observed in two types of experiments, with one representing a nearly free sliding interface and the other a strongly bonded interface. Interestingly, the AFM extrusion profiles seemed to contour with the local grain structures near the top of the via, suggesting that the grain structure not only affects the yield strength of the Cu and thus its plasticity but could also be important in controlling the pop-up behavior and the statistics for a large ensemble of vias. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4833020]

The through-silicon-via (TSV) is a critical element that provides short vertical interconnects in die stacks to improve the electrical performance, power consumption, and form factor for 3D integrated circuits. The mismatch of thermal expansion coefficients (CTE) between the Cu via and the Si wafer can induce significant thermal stresses that impact the device performance, raising serious reliability concerns.[1,2] Of particular concern is the Cu extrusion induced by thermal stresses, which can cause failure in the TSV and in the adjacent interconnect structures during fabrication or thermal cycling. This has generated great interest recently in studying the Cu extrusion or the "pop-up" phenomenon to optimize the fabrication process for improved yield and reliability.[3–6] In these studies, a number of extrusion mechanisms have been proposed, including plasticity, interfacial sliding, and diffusive creep. Most of the proposed mechanisms are indirectly deduced based on the extrusion behavior observed in TSVs subjected to annealing or thermal cycling. Damages induced by extrusion in the backend interconnect structures have also been observed and can seriously impact the structural integrity, but the mechanism is not well understood.

In this paper, we report the results from a study of the mechanism of Cu extrusion in TSV structures. We first summarize results from the synchrotron x-ray micro-diffraction to investigate the stress and plasticity characteristics of TSV structures. Using the high brightness of the synchrotron source, this technique has the unique capability to directly observe the local plasticity in Cu and the stress and strain distributions in the surrounding Si with submicron resolution.[7,8] The local plasticity observed at the Cu/Si interface near the top of the via plays an important role in inducing the non-recoverable plastic deformation that accounts for Cu extrusion during thermal cycling. This mechanism is confirmed by direct measurements of the extrusion of Cu vias after thermal cycling using atomic force microscopy (AFM). An elastic-plastic analysis is formulated to evaluate the effect of plasticity on the stress and extrusion behavior of the TSV. Based on this analysis, we are able to quantify and confirm that the observed Cu extrusion is consistent with the proposed plasticity mechanism. Moreover, the evolution of the Cu grain structure was found to be important in controlling the yield strength and thus the onset of the plastic deformation of the Cu TSV. This indicates a basic approach to minimize the Cu extrusion by optimizing the Cu grain structure through controlling the electroplating and the annealing processes in TSV fabrication.

The samples investigated in this study contained periodic arrays of blind Cu vias 10 μm in diameter and 55 μm in height built in a 780 μm thick (001) Si wafer. The TSV structure was fabricated by standard etching and electroplating processes incorporating 0.4 μm oxide and 0.1 μm Ta barriers. The wafer curvature technique was used to measure the stress behavior of TSV samples subjected to thermal cycling from room temperature (RT) to 200, 300, and 400 °C, respectively.[9,10] As shown in Figure 1, a nonlinear curvature behavior was observed during heating, which can be attributed to stress relaxation in Cu due to grain growth. During subsequent cooling, with the grain structure stabilized, the TSV

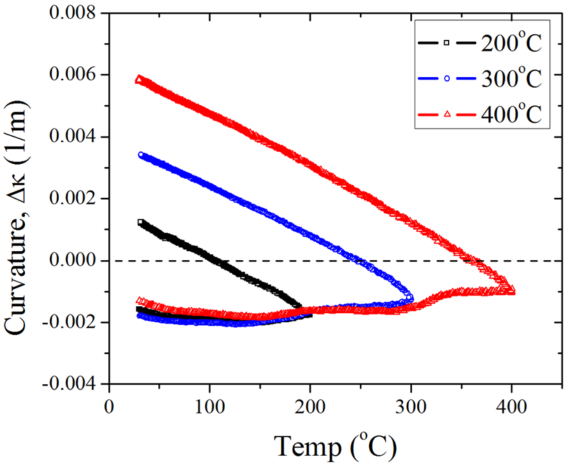

FIG. 1. Wafer curvature measurements for three TSV samples thermal cycled to 200 °C, 300 °C, and 400 °C, respectively.

exhibited a nearly linear elastic behavior, accumulating large residual stresses in both Cu and Si. The growth of the Cu grain size with thermal cycling temperature was measured by electron backscatter diffraction (EBSD) and found to increase from 0.9 μm as received to 1.1 μm, 1.2 μm, and 1.3 μm after cycling to 200 °C, 300 °C, and 400 °C, respectively.[9]

Scanning x-ray microdiffraction with polychromatic beam (white beam) was carried out on the cross-section of the TSV samples using Beamline 12.3.2 at the Advanced Light Source (ALS), Lawrence Berkeley National Laboratory (LBNL).[7] The x-ray microbeam scanning was performed at a step size of 1 μm/step with a beam size of $1\,\mu\text{m} \times 1\,\mu\text{m}$ and x-ray energies of 5 keV to 22 keV. Indexation of the observed Laue patterns was conducted for Cu and Si separately. Details of the measurement can be found elsewhere.[7–9]

For Cu, the shape of the Laue reflections was examined, and the change of the diffraction peak width of Cu near the top of the TSV before and after thermal cycling is shown in Figure 2. Compared to the as-received sample, an increase in the average peak width (APW) was observed in the Cu vias after thermal cycling to 300 °C and to 400 °C, concentrated in the area near the top of the vias. The asymmetric broadening of APW can be correlated to increased geometrically necessary dislocation density in Cu, indicating local plastic deformation.[11] In contrast, thermal cycling to 200 °C did not seem to induce broadening of the APW.

The APW broadening for grains near the top surface of the via provides a direct evidence of local plasticity. This is shown by the Laue reflections in reciprocal space for grains near the top of the via in Figure 3 where APW broadening was clearly observed after thermal cycling to 400 °C, but more faintly after thermal cycling to 200 °C. This suggests that local plasticity has occurred after thermal cycling to 400 °C, but not after thermal cycling to 200 °C. In addition, the reflection pattern appeared to split into multiple peaks as readily observed in the 3D contours, suggesting the formation of subgrains as a result of large plastic deformation.[9]

Results from the wafer curvature measurements show overall stress build-up in the TSV structure during thermal cycling while x-ray microbeam diffraction provided evidence of local plastic deformation near the top of the Cu via. Together, the stress build-up and plasticity lead to Cu extrusion or “pop-up” of the TSV top surface after thermal cycling, which was confirmed by AFM as shown in Figure 4. Comparing to the as-received sample, the Cu via thermal cycled to 200 °C was found to remain at 26 nm with no additional extrusion, which is consistent with the negligible peak broadening observed in Figure 2. For vias thermal cycled to 300 °C and to 400 °C, the top surface of the Cu via was found to extrude to an average height of 40 nm and 110 nm, respectively, which is also consistent with the measurement in Figure 2. Interestingly, the profile emerged to have a “donut” shape at 300 °C and continued to grow at 400 °C, which is in agreement with the observation in a previous study.[6] The AFM extrusion profiles seemed to contour with the local grain structures near the top of the via, particularly for the donut shape at 400 °C, suggesting that the local plasticity of individual grains near the top could be important in controlling the amount and the statistical distribution of via extrusion.[5]

The plasticity mechanism for Cu extrusion is illustrated by an elastic-plastic analytical model. Interfacial

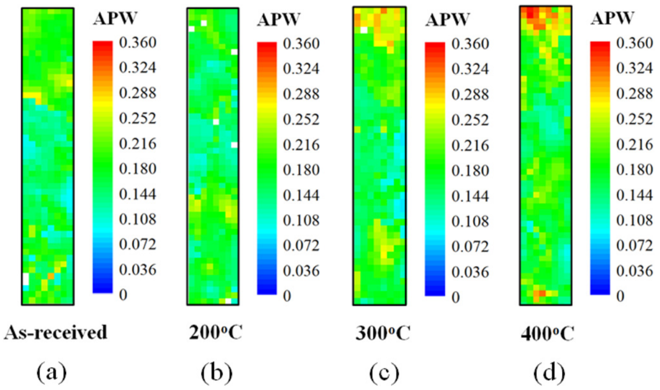

FIG. 2. APW of Cu in the TSV samples (a) as-received and after thermal cycling to (b) 200 °C, (c) 300 °C, and (d) 400 °C.

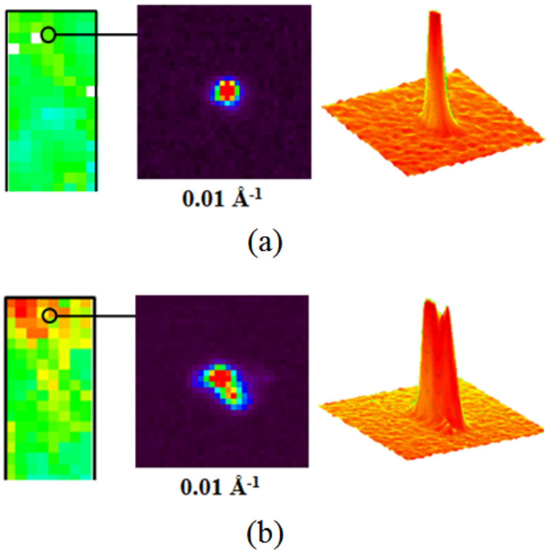

FIG. 3. Comparison of the (024) reflection shape for a grain near the top of the via (a) after 200 °C thermal cycling and (b) after 400 °C thermal cycling.

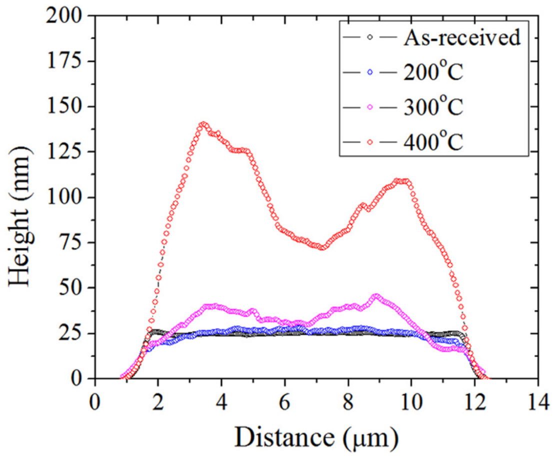

FIG. 4. Average via extrusion induced by thermal cycling from RT to 400 °C and measured by AFM. The extrusion heights are obtained by averaging measurements of 5 vias for each case.

delamination and Cu plasticity have been suggested as two possible mechanisms in previous studies.[12,13] Interfacial delamination could result in via extrusion at high temperatures, but very little extrusion remains after cooling if no plastic deformation occurred in the Cu via. To elucidate the effect of Cu plasticity, we assume a free sliding interface in the analytical model as an upper bound estimate for via extrusion. We first consider heating of a TSV from room temperature assuming zero initial stress before heating. The mismatch of thermal expansion between the Cu via and Si induces a biaxial compressive stress in the via upon heating with a thermal load of ΔT

$$\sigma_r = \sigma_\theta = -\Delta T(\alpha_{Cu} - \alpha_{Si})\left(\frac{1-\nu_{Cu}}{E_{Cu}} + \frac{1+\nu_{Si}}{E_{Si}}\right)^{-1}. \tag{1}$$

Here we have ignored the non-uniform stress distribution near the surface and assumed the materials to be linear elastic. The stress induces an elastic strain in the axial direction of the via, which results in an elastic extrusion relative to the thermal expansion of Si

$$\begin{aligned}\frac{\Delta H_e}{H} &= \varepsilon_{z,Cu} - \varepsilon_{z,Si}\\ &= \Delta T(\alpha_{Cu} - \alpha_{Si})\left(1 + \frac{2\nu_{Cu}}{E_{Cu}}\left(\frac{1-\nu_{Cu}}{E_{Cu}} + \frac{1+\nu_{Si}}{E_{Si}}\right)^{-1}\right),\end{aligned} \tag{2}$$

where H is the via height and ΔH_e is the elastic extrusion. The elastic extrusion increases linearly with temperature as $\Delta H_e = \beta_e H \Delta T$, with $\beta_e = 20.64$ ppm/°C by using the typical values for the thermomechanical properties of Cu and Si ($\alpha_{\mathrm{Cu}} = 17\,\mathrm{ppm/°C}$, $\alpha_{\mathrm{Si}} = 2.3\,\mathrm{ppm/°C}$, $E_{\mathrm{Cu}} = 110\,\mathrm{GPa}$, $E_{\mathrm{Si}} = 130\,\mathrm{GPa}$, $\nu_{\mathrm{Cu}} = 0.35$, and $\nu_{\mathrm{Si}} = 0.28$). If no plastic yielding occurs, however, the elastic extrusion would decrease with the same rate upon cooling and vanish at room temperature after a full thermal cycle.

On the other hand, assuming prefect plasticity with a yield strength of σ_y for the Cu via, plastic yielding is predicted when heating above a critical temperature

$$\Delta T_y = \frac{\sigma_y}{\alpha_{Cu} - \alpha_{Si}}\left(\frac{1-\nu_{Cu}}{E_{Cu}} + \frac{1+\nu_{Si}}{E_{Si}}\right), \tag{3}$$

which is proportional to the yield strength σ_y. Beyond the critical temperature ($\Delta T > \Delta T_y$), the Cu via deforms plastically. Since plastic deformation conserves volume, the volume of the Cu via changes only by thermal expansion as

$$\frac{\Delta V}{V} = 3\alpha_{Cu}(\Delta T - \Delta T_y). \tag{4}$$

Meanwhile, the thermal expansion of Si causes change of the via radius as

$$\frac{\Delta R}{R} = \alpha_{Si}(\Delta T - \Delta T_y). \tag{5}$$

As a result, the plastic extrusion can be predicted as

$$\frac{\Delta H_p}{H} = \frac{\Delta V}{V} - \frac{2\Delta R}{R} = (3\alpha_{Cu} - 2\alpha_{Si})(\Delta T - \Delta T_y). \tag{6}$$

Thus the plastic extrusion also increases linearly with temperature, but with a higher rate as $\Delta H_p = \beta_p H(\Delta T - \Delta T_y)$, with $\beta_p = 46.4$ ppm/°C. The plastic extrusion rate is over twice of the elastic extrusion rate, leading to significantly more via extrusion at high temperatures. Importantly, the plastic extrusion does not vanish after cooling, resulting in a non-zero residual extrusion after a full thermal cycle. The extrusion behavior deduced from this analytical model is shown in Figure 5 for thermal cycling from room temperature to 300 °C and 400 °C.

The effect of interfacial properties on Cu extrusion is further investigated by finite element analysis (FEA) using an axisymmetric model. The development of via extrusion during a thermal cycle is evaluated for two cases with different interfacial bonding characteristics, and the results are plotted in Figure 5 for comparison with the analytical model. First, a perfectly bonded interface is assumed between the copper via

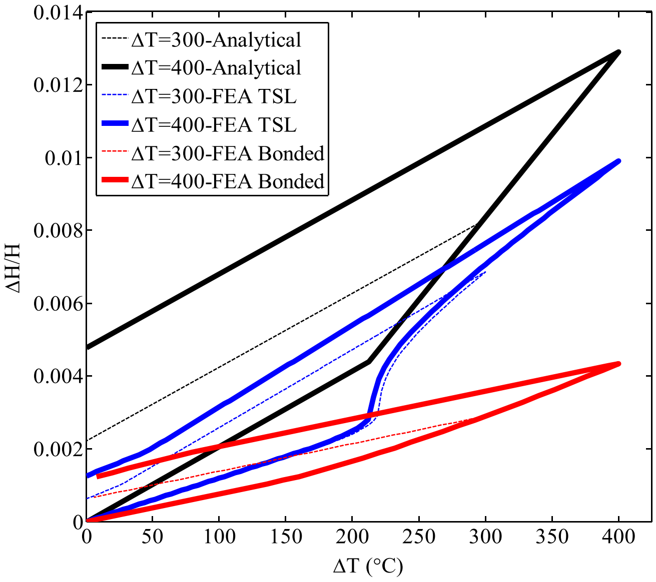

FIG. 5. Comparison of extrusion ratio between analytical and FEA results assuming interfaces with perfect bonding and bilinear traction separation relationship. Assume zero initial residual stress.

and silicon. With the perfect bonding, the extrusion is significantly reduced, by ∼3×, at room temperature and by a comparable factor also at maximum temperature. The results indicate that the effect of plasticity on extrusion is reduced by the interfacial bonding between the Cu via and silicon. In the second case, a cohesive interface model is assumed, represented by a bilinear traction-separation law (TSL) with an adhesion energy of 2.5 J/m^2 and a shear strength of 50 MPa. The via extrusions at both room and maximum temperatures are considerably higher than the bonded case although they are still lower than what the analytical model predicts. Hence, we conclude that the via extrusion depends on both Cu plasticity and interfacial bonding. We further investigate the effect of hardening in Cu plasticity on via extrusion and find that hardening has only a modest effect of less than 10%.

According to the analytical model, the magnitude of the residual extrusion after a thermal cycle depends on the highest temperature during thermal cycle and the plastic yield stress of the Cu via. Assuming no reverse yielding during cooling, the residual extrusion is predicted as

$$\Delta H_r = H(\beta_p - \beta_e)(\Delta T_m - \Delta T_y). \tag{7}$$

In Figure 6, the predicted residual extrusions deduced from the analytical and the FEA models are summarized for vias after cooling down to room temperature. Assuming a yield strength for Cu of 200 MPa, the critical temperature for plastic yielding is about 239 °C, as indicated in Figure 6, below which zero residual extrusion is predicted at room temperature. For comparison, the extrusion data reported in Ref. 6 and this study are included. Interestingly, while the data from this study seem to agree with the cohesive interface model, the extrusions reported in Ref. 6 are considerably higher, in reasonable agreement with the analytical model (free-sliding interface). This suggests that the TSV structures in that study may have a weaker interface, thus more prone to interfacial sliding and extrusion. We note that the overall agreement between the extrusion data and the model predictions depends on the material properties used in the model. For example, the extrusion reported in Ref. 6 can be in better agreement with the analytical model if the Cu yield strength is reduced.

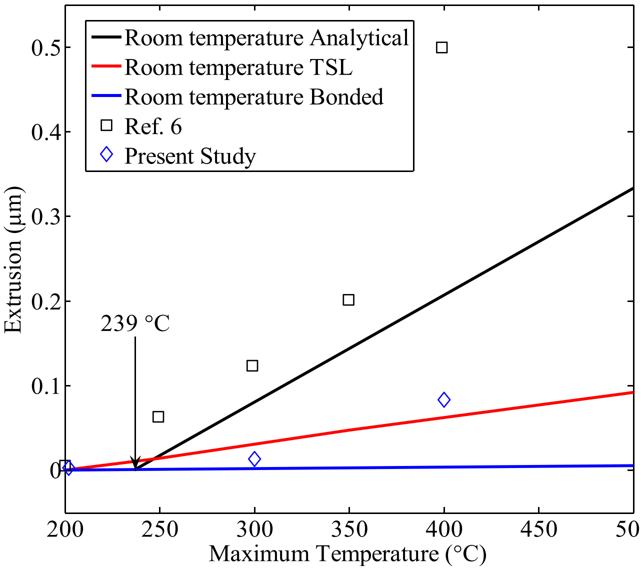

FIG. 6. Summary of the results for via extrusions at room temperature deduced from the analytical model and FEA models with interfaces characterized by rigid bond and TSL behavior. Included for comparison are data taken from this study and Ref. 6.

In summary, in this study of the via extrusion mechanism, we demonstrated the plasticity mechanism for Cu extrusion in TSV structure under thermal cycling. The local plasticity was directly observed by synchrotron x-ray microdiffraction at the top of the interface with the amount increasing with the peak thermal cycling temperature. The Cu extrusion was confirmed by AFM measurements and found to be consistent with the plasticity behavior. Elastic-plastic analyses were carried out based on analytical and FEA models with different bonding characteristics for the via/Si interface. The model predictions were able to account for the via extrusions observed in two types of experiments, with one similar to a free sliding interface and the other a strongly bonded interface. Interestingly, the Cu extrusion profile seemed to contour with the local grain structures near the top of the via, suggesting that the grain structure not only affects the yield strength of the Cu and thus the plasticity behavior, but could also be important in controlling the pop-up behavior and the statistics for a large ensemble of vias.

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