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Synchrotron X-Ray Microdiffraction Investigation of Scaling Effects on Reliability for Through-Silicon Vias for 3-D Integration

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***Abstract*—Synchrotron x-ray microdiffraction has been applied to TSV characterization in various studies for nondestructive inspection with submicron resolution due to its high beam intensity and penetration depth. In this paper, the application of this technique to TSV investigations is examined and the correlation of the plastic deformation to the microstructure and extrusion behavior along with the effect of TSV dimensional scaling is examined. It is shown that the variability of the copper microstructure and resulting TSV behavior requires a larger number of samples in order to report statistically significant observations. The role of the microstructure in creating statistical scatter is demonstrated through microdiffraction measurements of grain orientation correlated with the observed peak widening, which shows that degraded TSV reliability is largely due to the high elastic anisotropy of copper. After taking the statistical variations into account, the scaling effect was clearly observed, with larger plastic deformation in 2μm diameter TSVs than in 5μm diameter TSVs consistent with microstructure variations. This is confirmed by TSV extrusion measurements, which show that the magnitude and statistical spread of the via extrusion for the 2μm diameter TSVs is higher than that of the 5μm diameter TSVs. These results, validated by thermomechanical simulation, demonstrate first that large sample sizes are required in copper TSV investigations due to high variability, which is not improved with scaling.**

I. Introduction

Through-Silicon vias (TSVs) are a crucial technol-ogy for enabling full three dimensional integration of microchips, as well as for 2.5D packaging architectures using silicon (Si) interposers, which increase wiring density, improve package form factor, and reduce interconnect delay [1], [2]. However, copper (Cu) TSVs pose unique reliability risks due to the mismatch in the coefficient of thermal expansion between the Si and the Cu, causing thermal stress buildup and via extrusion, which degrade device performance and reliability [3], [4], [5]. Local plastic deformation near the top of the TSV has been shown to be a basic mechanism of via extrusion, and that the Cu microstructure is important in controlling the extrusion statistics [6], [7], [8].

Synchrotron x-ray microdiffraction has been used as a nondestructive technique to characterize the strain behavior for both the Cu and the Si surrounding TSVs [11], [12], [13]. This technique has unique capabilities with its high beam intensity to measure the stress tensor components with submicron resolution and to correlate local lattice deformations to grain orientations. In addition, the local plastic deformation in the Cu grains can be determined from the average Laue peak widening (APW), which occurs due to geometrically necessary dislocations (GNDs) induced by plastic deformation [6], [14]. These characteristics are microstructure dependent, particularly for Cu, which has high elastic anisotropy. However, such studies performed to date have employed small sample sizes lacking statistical significance.

In this paper, sample averaging method is applied to synchrotron x-ray microdiffraction to measure stress and local plasticity in Cu TSVs with variable grain structures. It is found that by averaging over a sufficient number of samples, the results can become statistically significant, making it possible to study the effect of microstructure and of scaling on the extrusion and reliability behavior of TSVs. In this study, the white beam microdiffraction is used in conjunction with electron beam back diffraction (EBSD) to correlate the stress behavior to the grain structures as a function of the TSV diameter. Although the average grain size is not found to be correlated to the TSV diameter, the extrusion is higher for the 2μm diameter TSVs than for the 5μm and 10μm TSVs. Similarly, the microdiffraction results demonstrate higher average APW for the 2μm diameter TSVs and thus experimentally confirm the correlation between plasticity and via extrusion. Since integrated circuit reliability is determined by the worst-case, i.e., the weakest link, TSVs with the earliest failure rates, this paper further investigates the role of the microstructure in the extrusion statistics and uses statistical microdiffraction results to find that the mechanism is strongly correlated to the microstructural parameters.

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The microdiffraction study was further supported by thermomechanical simulations demonstrating the effect of the anisotropic microstructure on the stress and extrusion behavior. The simulation showed ample effects of the scattered values for grain size and orientation, which evolve due to the strain energy-driven abnormal grain growth and are remarkably enhanced by the elastic anisotropy of Cu. This emphasizes the need for statistically significant correlations of Cu TSV studies with microstructure characteristics. Since the Cu microstructure evolution is difficult to control and is not stable under annealing, it seems that via extrusion and its variability will degrade TSV reliability with continued scaling.

II. Experimental Methods

The x-ray microdiffraction was performed at beamline 12.3.2 at the Advanced Light Source, Lawrence Berkeley National Laboratory. The samples were mounted at a 45° angle from the incident beam and from the detector, and white beam (5-22 keV) scans were performed at room temperature. The observed Laue patterns were analyzed using x-ray microdiffraction analysis software (XMAS) to extract orientation, strain, and peak data relating to plastic deformation in individual grains [15].

Two sets of electroplated Cu blind via arrays are investigated, one set with 2μm $\times$ 40μm TSVs and another with 5μm $\times$ 50μm TSVs, and a via pitch of 20μm for both. These two sample sets were fabricated with similar etching and filling processes, and a third set of TSVs from another supplier that measured 10μm $\times$ 55μm, with a pitch of 40μm in the x-direction and 50μm in the y-direction was also included in the study for comparison. All three TSV types were fabricated with the via middle process. Samples were prepared for electron backscatter diffraction (EBSD) by mechanical polishing and focused ion beam milling to finish the via surface. In contrast, the x-ray microdiffraction measurements were performed on a cross-sectional surface that does not expose the Cu via, and thus minimized the adverse effects of sample preparation on Cu.

III. Microdiffraction and Simulation Results

Initial white beam microdiffraction measurements of the lattice strain in the 2μm and the 5μm diameter TSVs show high variability within each TSV and between TSVs. The von Mises stresses (Fig. 1) show large local variations in the Cu stress states for all diameters, which are due to scattered grain sizes and orientations which are induced by the high elastic anisotropy of Cu. This result agrees with TSV measurements published elsewhere where there are large deviations in measured lattice strains for a sufficient sample size.

The APW results, which measure local plastic deformation, also exhibit large data scatter overall, as shown in Fig. 2a for the 2μm and the 5μm diameter TSVs. Shown in Fig.2b is the correlation of APW to grain orientation. Upon close examination, there is a good correlation of the variations in the APW results with the microstructure distribution where the highest APW values are mainly associated with the grain boundaries between (111)-type grains and (100)-type grains. This indicates that local plasticity is induced near certain types of grain boundaries due to the discontinuities in the thermomechanical properties because of Cu's high elastic anisotropy.

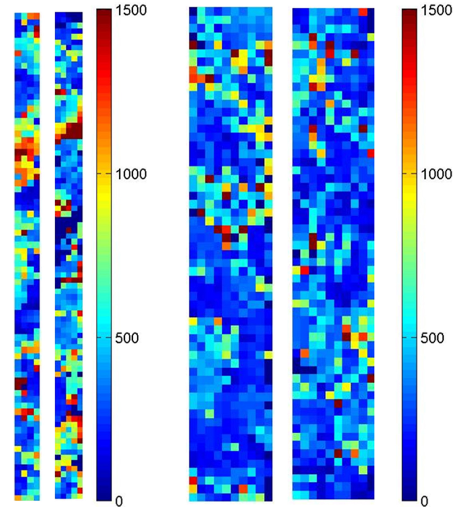

Fig. 1. Von Mises stresses (MPa) calculated from the lattice strain measured via synchrotron x-ray diffraction. Variability is apparent for both the 2μm (left) and 5μm (right).

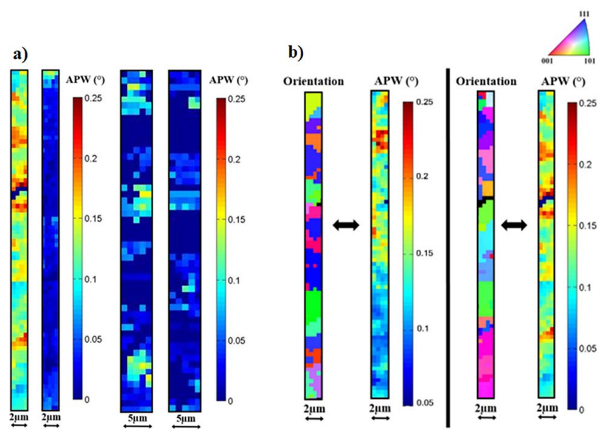

Fig. 2. (a) Variation in APW for 2 and 5μm TSVs. (b) Correspondence of APW to orientation.

The overall statistical correlation of APW with the Cu grain structure was quantified using a sample averaging technique. The results for 2μm, 5μm and 10μm TSVs obtained by averaging at least 6 vias for each diameter are shown in Fig. 3a. After sample averaging, the overall scaling effect on local plasticity becomes clear, where the average APW and standard deviation are higher for the 2μm diameter TSVs. The APW and its statistical deviation integrated over the first 5μm in the TSV are shown in Fig. 3b, where the 2μm diameter TSVs show higher measured extrusion heights and higher statistical scatter than the 5μm diameter TSVs.

Representative TSV microstructures, which were all annealed further to 400° C, are plotted in Fig. 4 to trace the root causes of the observed results. Microstructures were measured via EBSD and the orientations are plotted with respect to the in plane radial direction. Abnormal grain growth is seen in all the TSVs, increasing the statistical scatter and microstructure instability. This phenomenon is driven by strain energy minimization and thus worsens with additional annealing [16]. The average grain sizes and textures do not scale with

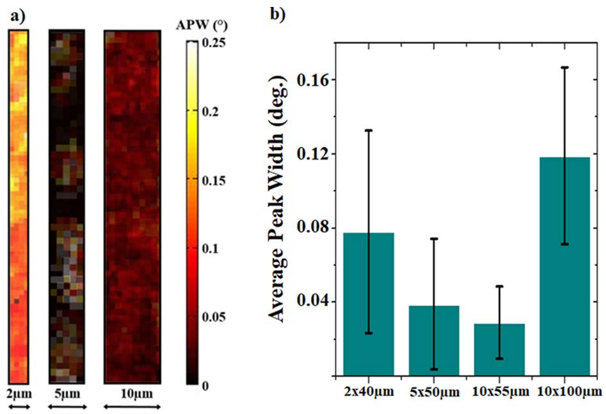

Fig. 3. a) Maps of averaged APW results for various TSV sizes and b) bar chart of average APW with standard deviations.

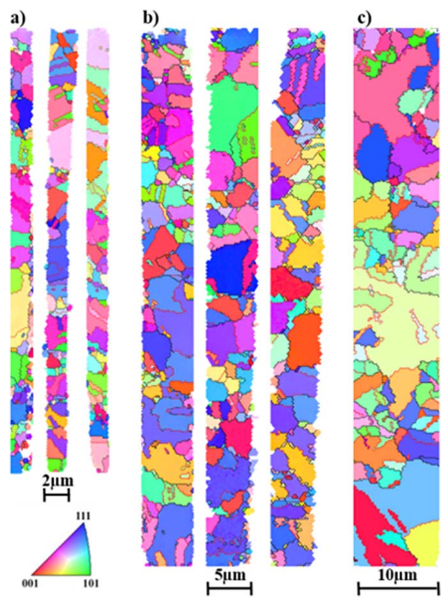

Fig. 4. Microstructures resulting from a 400° C anneal for the (a) 2μmx40μm TSV, (b) 5μmx50μm TSV, and the (c) 10μmx55μm TSV.

TSV diameter, indicating that the fundamental grain growth mechanism does not scale in this diameter range, but the 2μm diameter TSVs uniquely demonstrate large sections of bamboo-like microstructures and the maximum grain size of the 2μm diameter TSVs is higher than that of the 5μm diameter TSVs. This microstructure scaling effect confirms the APW and extrusion measurements that indicate worsened statistical reliability for the 2μm diameter TSVs.

The effect of the microstructure on the extent of the plastic deformation and extrusion with scaling can be further demonstrated with thermomechanical simulation by finite element analysis. The anisotropic microstructure and plasticity have been shown to be crucial to understanding TSV reliability and must be included in the simulations in order to account for the statistics of TSV stress and extrusion. EBSD data was used to recreate the microstructures of the top 5μm of two 2μm diameter TSVs and two 5μm diameter TSVs, while the rest of the TSV is represented with an averaged, isotropic Cu. The plastic strains in the axial direction are plotted for a 400° C annealing cycle. The derivation of the simulations and the results are shown in Figs. 5 and 6 for the 5μm and 2μm TSVs,

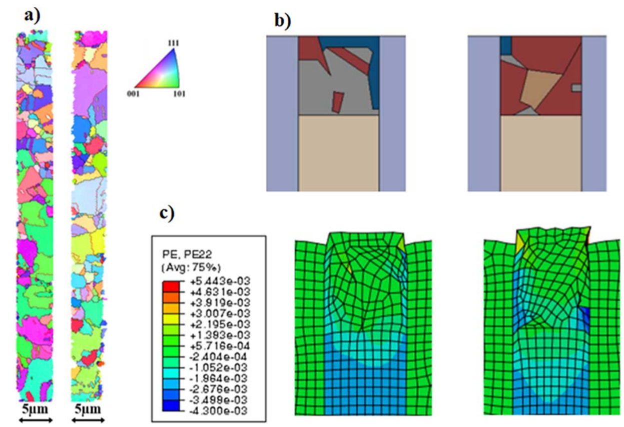

Fig. 5. Microstructures resulting from a 400° C anneal for the (a) 2μmx40μm TSV, (b) 5μmx50μm TSV, and the (c) 10μmx55μm TSV.

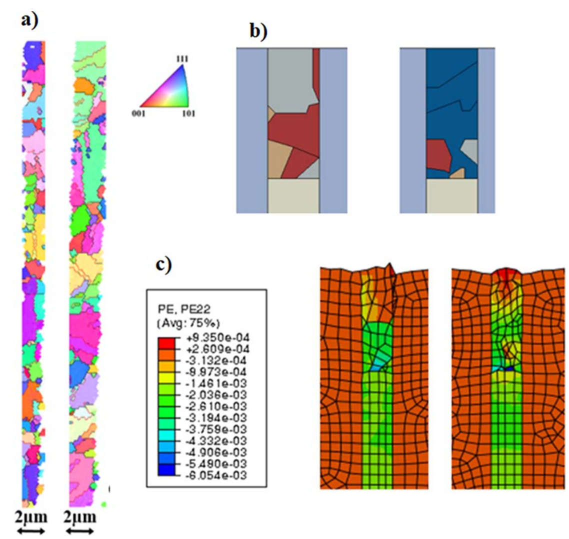

Fig. 6. (a) Grain structure for 2μm TSVs, (b) transcribed grain structure for simulation and (c) resulting plastic strain in the axial direction.

respectively. These plots demonstrate that the grain structure largely determines the thermomechanical response. Simulation results for an isotropic model are smooth and symmetrical, but the addition of anisotropic Cu grains causes significant local variations in the stress and plasticity, similar to the microdiffraction results of this study, as well as inducing irregular deformations that texture the TSV top surface, as has been reported in previous studies [17], [18].

IV. Summary

In this paper, the application of microdiffraction to TSV characterization is examined, and the effect of down scaling TSV dimensions on the extrusion mechanisms is investigated using white beam synchrotron x-ray microdiffraction combined with further experiments and thermomechanical simulation. Variability in Cu TSVs is found to require larger sample sizes, and thus the plasticity mechanism is investigated through sample averages of the APW, which is a measure of the GND density due to plastic deformation. This is correlated to the extrusion behavior and to the local microstructure parameters, and downscaling is shown to worsen the reliability statistics due to the elastic anisotropy of Cu, which promotes abnormal grain growth and thus scatter in the grain sizes and orientations.

Microdiffraction results demonstrate that the magnitude and deviation of the APW increase with scaling and that the APW representing the local plasticity is correlated to the microstructure. EBSD measurements reveal that the average grain size does not scale closely with TSV diameter, implying that while the grain growth mechanism is not sensitive to the TSV dimensions in this study, there are fewer grains across the TSV diameter as scaling continues. The microstructure evolution is driven by the elastic anisotropy of Cu, where the (100) orientation is favored by the strain energy while the (111) orientation is preferred by the surface energy [19]. This competition under annealing gives rise to the random textures and twins observed, while the strain energy induces abnormal grain growth, which increases microstructural scatter. This is confirmed in the extrusion results, where the variability is high, and the unique microstructure of the 2μm diameter TSVs yields the highest extrusion values and scatter. The statistical correlation between the microstructure and the extrusion is demonstrated experimentally in the microdiffraction measurements where the APW varies with the Cu grain boundaries. The thermomechanical models validate these results, showing that the introduction of microstructural characteristics yields non-uniform stress and deformation patterns, especially at boundaries between dissimilar grains.

Several previous studies have shown that grain boundaries induce local stress state variations, especially in an anisotropic material such as Cu, where the mechanical properties are discontinuous across the grain boundaries [20], [21], [22]. This phenomenon is directly observed in this study by microdiffraction and is extended to the local plasticity in the individual grains, and thus to the extrusion behavior. Post-plating annealing and additional thermal cycles increase the strain energy in the TSV, which both favors the (100) orientation and induces further abnormal grain growth, leading to increased statistical scatter in the extrusion data [16].

Since the via middle process requires further high temperature annealing, it is likely that Cu TSVs will continue to present reliability issues, due to this instability in the Cu microstructure under annealing, which creates difficulty in controlling the worst case TSVs. The impact of the increased dislocation density in the 2μm diameter TSVs, evidenced by the APW measurements, requires further study of its contribution to the extrusion mechanism. Nonetheless, the statistical microdiffraction results clearly confirm that due to the anisotropy of Cu, the microstructure of Cu and the statistical variability must be considered in evaluating Cu interconnect behavior at any size scale.

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