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ASME Paper Title: Microstructural Evolution and Protrusion Simulations of Cu-TSVs Under Different

Loading Conditions

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ASME Journal Title: Journal of Electronic Packaging

Date of Publication (VOR* Online)

Volume/Issue 142(1) 10/10/2019

<https://asmedigitalcollection.asme.org/electronicpackaging/article/doi/10.1115/1.4044648>

ASME Digital Collection URL: crostructural-Evolution-and-Protrusion

DOI: <https://doi.org/10.1115/1.4044648>

*VOR (version of record)

Simulations on microstructural evolution and protrusion of Cu-TSVs under different loading conditions

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Thermal stress-induced protrusion of copper through-silicon-vias (Cu-TSVs) during the thermal processing poses serious reliability concern in three-dimensional system integration. In this study, a phase-field-crystal model is used to investigate the protrusion and the microstructural evolution of blind Cu-TSVs under different loading conditions. The protrusion is only observed when the TSV is under ϵ_x , ϵ_y and γ_{xy} . No protrusion is observed when TSV is subjected to a pure shear strain γ_{yx} . The simulation results suggest that the grains in the top layer of the TSV contribute more to both the protrusion profile and level of protrusion height than the grains below. The protrusion is larger when the misorientation between the grains is larger and the grain size along the y-direction is smaller. In addition, a phenomenological model linking protrusion and microstructure factors, and a visual guide from the viewpoint of plastic flow are provided to understand the origins of Cu-TSV protrusion.

1 Introduction

Nowadays, the development of artificial intelligence (AI) gives new vitality into the advanced electronic packaging technology. Three-dimensional (3D) devices, e.g., s-stacking high bandwidth memory (HBM), is expected to keep up with the increasing requirement of packaging density [1]. In realizing 3D packaging, an important idea is to utilize a through-silicon-via (TSV) technology [2–4]. However, the mismatch of coefficients of thermal expansion between the normal filler material Cu and the surrounding silicon frequently leads to protrusion when the TSV structures are subjected to thermal processing [5]. This causes damages to the back-end-of-line (BEoL) layers and thus the failure of 3D packaging, posing a serious reliability issue to be solved.

To provide better understanding of the root cause protrusion, the strain or stress state in the TSVs needs to be determined. There are a few experimental studies in the literature attempting to analyze the stress in the TSVs. Nano-indentation is used by Che *et al.* to measure the residual stress in the TSV [6]. Okoro *et al.* measured the stress of the TSVs of different size using micro-Raman spectroscopy [7]. Liu *et al.* used synchrotron X-ray microdiffraction to mea-

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sure the microscale thermomechanical strain in-situ [8].

In addition, the microstructure of polycrystalline Cu is a significantly important factor that needs to be considered to fully understand the random nature of the TSV protrusion. Jiang *et al.* used an electron back-scattered diffraction (EBSD) technique to show that larger grains were found in TSVs under thermal cycling with a higher peak temperature [9]. Recently, a large ensemble of Cu-TSV protrusions was examined and a statistical model correlating the protrusion height and the number of grains near the TSV top end was established, which showed more grains resulted in a higher protrusion [10]. Due to the random nature of the polycrystalline Cu, it is difficult to find a direct relationship between the grain structures and protrusion. The most frequently used method to characterize the grain structures in TSVs is to measure an average grain size. However, the average grain size is far from enough to characterize the microstructure of Cu-TSVs. To address this issue, simulation methods considering controllable atomic-scale structures can provide direct microstructural information. In a recent work, we reproduced the process of Cu protrusion of TSV using a phase-field-crystal (PFC) model, revealing the microstructural evolution accompanying the protrusion process at the atomic scale [11]. PFC models have been applied to simulate the phenomena in material science with atomic spatial scale and diffusive time scale resolutions, such as nucleation and polycrystalline solidification, heteroepitaxial growth, and structural phase transformations [12, 13]. In addition, PFC models can capture elasticity and plasticity phenomena relevant to solid-state processes such as dislocation creation and annihilation, dislocation motion, and creep [14, 15].

In this study, we use the PFC model to simulate the microstructural evolution and protrusion of Cu-TSVs under different loading scenarios and depict a general picture of TSV protrusion in relation to the microstructure and loading conditions. The rest of the paper is organized as follows. First, the PFC model is briefly introduced. Second, the effect of different loading conditions on Cu-TSV protrusion is discussed. Meanwhile, the protrusion behavior of TSVs with different grain structures and loading distributions is investigated in detail. Finally, a general picture to understand the TSV protrusion is discussed.

2 Method

Using a two-point correlation function, a two-mode PFC model has been developed to simulate a square lattice in two dimensions [16]. In the PFC model, an order parameter ρ , which has the form of a plane wave with the same periodicity as the lattice, is introduced to represent the local time-averaged atomic density of a material system. In the 2D case, the two-mode order parameter is written as [16]:

$$\rho = \bar{\rho} + A[\cos(qx) + \cos(qy)] + B\cos(qx)\cos(qy) \quad (1)$$

where A and B are related to the amplitudes of two sets of density waves. $q = 2\pi/a$ is a parameter related to the lattice

constant a . The order parameter ρ can mimic a square lattice, which corresponds to the $\{100\}$ crystallographic plane of Cu. Moreover, the symbol $a = 0.25$ nm is defined hereinafter as the lattice constant of the Cu. Then, the free energy of the system is written as [16]:

$$F[\rho] = \int d\vec{r} \left\{ \frac{\rho}{2} [r + (\nabla^2 + 1)^2 (\nabla^2 + Q^2)^2] \rho + \frac{\rho^4}{4} \right\} \quad (2)$$

where $r = c(T - T_m)/T_m$ is the scaling temperature and $Q^2 = 2$ is a constant. Based on the variation in the free energy F of the system with respect to the order parameter ρ , the microstructural evolution is obtained by solving the governing equation [16, 17]:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \frac{\delta F}{\delta \rho} \quad (3)$$

In this study, a 2D-PFC model is adopted for computational efficiency. Fig. 1 shows the model configuration of our TSV structure. The edges of the TSV are marked out by solid gray lines. Noted that a trapezoid TSV is chosen because of the tapered nature of a drilled via [18], and the geometry effect was studied in our previous work [19]. The atomic-scale microstructure is developed by placing crystal nuclei inside the TSV and then initiating solidification. Then, the microstructure is further equilibrated until it remains unchanged. To apply a loading, external layers are added to surround the TSV. The top layer is set as a grain with a 0° orientation, providing a solid cover for the TSV. In the PFC model, the loading is applied by introducing a “penalty term” to the free energy with the form [20]:

$$F[\rho]' = F[\rho] + \int d\vec{r} M(\vec{r}) [\rho(\vec{r}, t) - \rho(\vec{r}(\vec{v}, r), t)] \quad (4)$$

where $M(\vec{r})$ is nonzero only in the external layers, except for the top cover layer. Motivated by the “penalty term”, the atoms inside the external layers are forced to move with a predetermined velocity $\vec{v}$ in a direction defined by the arrows, forming an angle θ with the horizontal line, as demonstrated in Fig. 1. Other parameters used in the PFC model are set as $(r, \bar{\rho}, A, B, q, |\vec{v}|) = (-1, 0.59, -0.31, -0.14, 1.0, 1.0 \times 10^{-4})$. The model parameter $r = -1$ fixes the system temperature to be approximately 700°C , as discussed in our previous study [21]. In experimental work, an annealing process of Cu-TSVs under the temperatures around $400 - 450^\circ\text{C}$ is usually carried out and results in Cu protrusion [10, 22–24]. In our simulation, the temperature is increased to accelerate the protrusion process. Despite of an increase in temperature, the mechanism of Cu protrusion remains the same [21], as molecular dynamics simulations suggesting that diffusional creep is the dominant mechanism in the temperature range between 327°C and 827°C in nanocrystalline metals [25, 26]. Noted that the length and time scales in the original PFC model and this study are dimensionless. In addition, the

Fig. 1: The PFC model configuration of a TSV structure. The edges of a trapezoid TSV are outlined by solid gray lines. Three layers of grains in TSV are marked out. The parallel arrows indicate the direction of the loading applied to the TSV, which form an angle θ with the horizontal line. The corresponding strain state of a material point in the TSV is shown in the illustration on the left side. Defect atoms in the TSV are highlighted by the yellow dots.

atoms in or near the grain boundaries (GBs) and dislocations in the TSV are defined as defect atoms, as highlighted by the yellow dots in Fig. 1. In order to study the effect of the grain structures in different regions of the TSV, we classified the grains in the TSV as grains in the top, middle and bottom, shown in Fig. 1. In particular, the two grains in the top layer shown in Fig. 1 are referred to grains 1 and 2 hereinafter.

3 Results and discussion

Due to the random nature of Cu grain structures after electroplating, it is difficult to measure the strain states in the TSVs for all possible microstructural configurations by experiments. Therefore, a PFC model is used here to simulate the microstructural evolution and protrusion behavior of Cu-TSVs under different loading conditions. The symbols ϵ_x , ϵ_y , γ_{xy} and γ_{yx} as shown in Fig. 1 are referred to as the components of the strain state of a material point in the TSV, which can be controlled by changing the boundary condition of the PFC model, i.e., the “penalty term”. Meanwhile, a systematic variation of the direction of loading θ , shown in Fig. 1, can represent all the strain scenarios of ϵ_x and γ_{xy} that the TSV could be subjected to. As an example, the loading with $\theta = 180^\circ$ means a compressive strain ϵ_x to the TSV, while the loading with $\theta = 150^\circ$ represents the combination of a compressive strain ϵ_x and a shear strain γ_{xy} . Noted that the loading is assumed to be uniformly distributed along the edges of the TSV for simplicity.

3.1 Under pure shear strain γ_{yx}

When the TSV is under pure shear strain γ_{yx} , the microstructural evolution was presented in our pervious study [19] and no protrusion was observed. In this case, the dislocations were found to move to the left and right edges of the TSV following the shear direction. As a result, glide steps were formed at the edges of the TSV. In addition, the atoms are found to diffuse in x -direction. The deformation of the TSV could only be found in the left and right edges and no protrusion out of the top surface can be observed. Therefore, TSVs under pure shear strain γ_{yx} lead to no protrusion and will not be discussed further in the following sections.

3.2 Under normal strain ϵ_x and shear strain γ_{xy}

The relationship between the TSV protrusion and the direction of loading is plotted in Fig. 3, with θ changing systematically from 0° to 360° . The curve shows that the mean protrusion increases then decreases with the increasing θ in general, with the maximal mean protrusion occurring at $\theta = 150^\circ$. The mean protrusion is calculated by averaging the height of the protrusion profile. For $\theta \leq 90^\circ$ and $\theta \geq 270^\circ$, the TSV is subjected to the tensile strain ϵ_x and shear strain γ_{xy} but little protrusion is produced, as shown in Fig. 2. Driven by the tensile strain ϵ_x , the atoms are forced to move to the edges of the TSV along the x -direction and the GB network in the TSV thickens. In particular, the thickness of GBs along the y -direction are found to increases more than other directions, e.g., GB1 is thicker than GB2 as shown in Fig. 2b. Moreover, the dislocations are observed to move to the left and right edges. As an end result, glide steps are formed in the edges but little protrusion is produced. Under the compressive strain ϵ_x and shear strain γ_{xy} , i.e., when θ is in the range of $90^\circ < \theta < 270^\circ$, e.g., $\theta = 150^\circ$ as shown in Fig. 1 and its final protrusion profile shown in Fig. 4a, the atoms near the left and right edges are found to diffuse inwards to the center of the TSV due to the symmetry of both the geometry and loading condition of the model settings. However, there is no destination to accommodate those diffusing atoms so that they are forced to diffuse in the y -direction and finally lead to protrusion. In order to show the protrusion behavior more clearly, we fixed the direction of loading $\theta = 150^\circ$ for the simulation in Section 3.2. Meanwhile, the microstructure of Cu significantly influences the behavior of TSV protrusion. The effect of different grain structures, i.e., grain size, grain orientation and grain size distribution will be investigated in the following sections.

3.2.1 Grain structures

Fig. 4 shows the protrusion profiles of three TSV samples with different grain structures. The initial microstructure of Fig. 4a and Fig. 4b contains the same grains 1 and 2 in the top layer, while the grains below are different. The resulting protrusion exhibits a similar two-peak profile, sketched by the black dashed curve, directly produced by the grains 1 and 2. In contract, as shown in Fig. 4c, three grains in the top layer leads to a different protrusion profile. The difference lies in that the grain 3 produces little protrusion.

Fig. 2: The microstructure of Cu-TSV under tensile strains: (a) $\theta = 60^\circ$ and (b) $\theta = 300^\circ$. The white arrows indicate the direction of loading and the black dotted ellipses mark out GB1 and GB2.

Fig. 3: The plot of protrusion versus the direction of loading θ .

Furthermore, twenty TSV samples with random initial grain structures are studied and the data of mean protrusion are calculated and plotted in Fig. 5. Amongst these samples, ten of them contain the same two grains in the top layer, while the rest three grains. It can be seen that the protrusion height scatters around the same level when the grains in the top layer remains the same. This result suggests that the protrusion behavior is more closely related to the grains in the top layer than below. Therefore, we focus our attention on the grains in the top layer in the following section. In addition, the protrusion profiles are found to remain similar as long as the grains in the top layer keep unchanged.

3.2.2 Grain size

As shown in Fig. 5, lower level of protrusion is found in TSVs with the top layer containing more grains, i.e., a smaller grain size along the x -direction. An experimental study by Messersmaecker *et al.* showed that the protrusion height was related to the number of grains at the top of the TSV and more grains led to a higher protrusion [24]. This seems to contra-

Fig. 4: The protrusion profiles of three TSV samples with different grain structures under the loading direction $\theta = 150^\circ$.

Fig. 5: The mean protrusion height of twenty TSV samples. Noted that the samples are prepared by keeping grains in the top layer unchanged while generating random grain structures below. The loading with $\theta = 150^\circ$ is then applied to the samples to observe the protrusion behavior.

dict to our simulation result. In fact, the protrusion behavior is not only influenced by the grain size, but also the loading condition. Here, the loading $\theta = 150^\circ$ considers only ϵ_x and γ_{xy} . When ϵ_y is also considered, the simulation results will

agree with experiment. Discussion on the combined effect of ϵ_x , ϵ_y , and γ_{xy} will be presented in Section 3.3.

Fig. 6 shows three TSVs of different grain size along the y -direction, with the number of grains in the top layer remaining the same. The size of grains 1 and 2 decreases gradually, i.e., the initial grain size approximately $30a$, $27a$ and $22a$ for Figs. 6a-6c, respectively, while the size of grains in the bottom layer increases accordingly. The resulted protrusion is found to increase gradually. More data of the mean protrusion height versus the grain size are plotted in Fig. 7. In a smaller grain, the diffusion of atoms is faster, as explained by the mechanism of creep in our previous study [21]. The rate of creep deformation can be described by the relationship: $\dot{\epsilon} \propto (\frac{1}{d})^p$. d is the average diameter of the grains and p is a power index associated with the kind of mechanism of diffusional creep. A smaller grain size means a higher rate of creep. As a result, a higher protrusion of the TSV with smaller grain size results.

In general, under the loading condition of ϵ_x and γ_{xy} with $\theta = 150^\circ$, a larger grain size along x -direction and a smaller grain size along the y -direction leads to a higher level of protrusion.

3.2.3 Grain size distribution in x -direction

In the above sections, the size distribution of grains 1 and 2 in the TSV keeps almost the same. However, a grain size distribution in the top layer of the TSV also influences the protrusion behavior. Two grains with different size ratios along the x -direction are placed in the top layer of TSV as shown in Fig. 8, i.e., 1:1 in Fig. 8a, 2:1 in Fig. 8c and 1:2 in Fig. 8e, respectively. The corresponding protrusion profiles are shown in Figs. 8b, 8d and 8f. The maximum protrusion is found for the ratio of 1:1 as shown in Fig. 8b. It can be observed that the GB between grains 1 and 2 remain the same position in Fig. 8b, while the GB is found to migrate in Fig. 8d and 8f. This phenomenon can be explained by the mechanism of Ostwald ripening: larger grains are more energetically favorable than smaller grains [27]. In Fig. 8d and 8f, the larger grain is more favorable and tends to grow even larger finally. With the GB migration, the applied strain to the TSVs can be alleviated and thus resulting in a lower protrusion. This result suggests that a symmetrical grain structure under a symmetrical loading will lead to a higher protrusion.

3.2.4 Grain orientation

In addition to the grain size, the grain orientation in the top layer also influences the TSV protrusion behavior. The orientation of grains 1 and 2, shown in Fig. 1, is systematically varied from 10° to 80° with an interval of 10° : the orientation of one grain, e.g., α of grain 1 or β of grain 2, is changed from 10° to 80° , while the orientation of the other grain remaining unchanged. The relationship between the misorientation between grains 1 and 2, i.e., $\eta = |\alpha - \beta|$, and the corresponding protrusion height is plotted in Fig. 9. The result shows that protrusion tends to be larger when the misorientation is larger. This is because the mobility of the GB

Fig. 6: The protrusion profiles of three TSVs with the grains 1 and 2 in the top layer varying size in the y -direction under the loading direction $\theta = 150^\circ$.

Fig. 7: The plot of mean protrusion versus the size in the y -direction of the grains 1 and 2 in the top layer.

decreases as the misorientation between the grains increases [28]. A lower GB mobility means that it is more difficult for the GB to migrate and accommodate the applied loading to the TSV. The deformation of the TSV ends up with directly pushing the grains out of the TSV surface, thus resulting in substantial protrusion. In addition, a misorientation

Fig. 8: The initial grain structure of three TSV samples. The size ratios along the x -direction between the grains 1 and 2 are 1:1 in (a), 2:1 in (c) and 1:2 in (e). The corresponding protrusion profiles are shown in (b), (d) and (f), respectively.

of around 60° is found to protrude most. This special GB is referred to as a twin boundary and it has been proved that a twin boundary has a higher creep resistance than other GBs and exhibits the highest stability and lowest mobility [29].

Fig. 9: The relationship between the mean TSV protrusion and the misorientation between the two grains in the top layer.

Further work focusing on the effect of twin boundaries and their interaction on the TSV protrusion behavior is currently undergoing.

3.3 Under normal strain ϵ_y

When the strain ϵ_y is applied to a TSV, two situations are considered here: pushing the grains at the bottom upwards or pulling the grains in the top layer out of the top end, as illustrated in Figs. 10a and 10c. First, the strain ϵ_y , i.e., under a compressive strain, is applied to the bottom by adding an external layer below the TSV, as shown in Fig. 10a. The corresponding initial microstructure is referred to Fig. 1 and the protrusion under this condition is negligible. It is noted that there are three layers of grains stacked along the y -direction in the TSV, such that the deformation of the grain in the bottom layer is difficult to be transferred to the top layer. When ϵ_y is applied, dislocations are found to emit from the bottom edge due to local deformation, and then annihilate with each other or at the neighboring GBs. The GBs act as sinks and absorb the dislocations. Therefore, the deformation of the grains in the bottom layer is rapidly reached an equilibrium state once again by little adjustment of the grains in the middle layer. Therefore, the deformation of grains in the bottom layer has little effect on protrusion. In contrast, if the strain ϵ_y is applied directly to the top end of the TSV, i.e., under a tensile strain, the protrusion will be larger, e.g., bumping up in the middle of the top surface, as demonstrated in Fig. 10c. Larger protrusion is produced because there is no buffer grains for the deformation. The protrusion in Fig. 10c shows a three-peak profile, with the grain in the middle also producing protrusion. The protrusion profile is found to contour with the local grain structures in the top layer, as reported by Jiang *et al.* [23].

Moreover, considering the ϵ_y , the results in Fig. 5 can be updated, as shown in Fig. 11. The protrusion height also scatters around the same level when the grains in the top layer remains the same. More grains in the top layer leads to a higher protrusion, which agrees with the experimental work of Messemaker *et al.* [24]. From the simulations of TSV protrusion under different loading conditions, a conclusion can be made here: with the same grain structure, different

Fig. 10: Different types of loading, as indicated by the white arrows, and the resulting protrusion profiles. (a) Loading applied at the bottom edge of the TSV resulting in little protrusion, (b) loading applied at the left and right edges of TSV producing a two-peak protrusion profile, and (c) loading applied at both the edges and the top end of TSV resulting in a three-peak protrusion profile.

loading conditions can lead to different levels of protrusion height and profiles.

3.4 The distribution of loading

As discussed above, the TSV protrusion is significantly influenced by the grain structures and the loading conditions. The applied loading in the above sections is uniform along the edges of the TSVs. However, the results from FEM simulation and experimental work reveal that strains in the TSVs exhibit heterogeneous distributions, i.e., a nonlinear distribution with higher strains occurring near the top end of TSVs [6, 30]. To further investigate the protrusion behavior, nonuniform distributions of loading should be considered. The distribution of loading is controlled by varying the strain rate $|\dot{\epsilon}|$ in different regions along the TSV edges. Detailed model configurations are summarized in Table. 1, and

Fig. 11: The mean protrusion of twenty TSV samples when considering ϵ_y . Noted that the samples are prepared by keeping grains in the top layer unchanged while generating random grain structures below.

the corresponding results are shown in Fig. 12. First, comparing M2 with M3, the protrusion is almost the same for the two TSVs, which suggests that the loading variation in the bottom region exerts little effect on protrusion. Then, comparing M3 with the TSV shown in Fig. 4a, the protrusion profiles also show a similar character. Finally, when examining M1 and M4, it can be observed that the protrusion is much smaller compared with other TSVs. This suggests that the loading applied near the top end of the TSV plays a greater effect on protrusion. A larger loading applied near the top end results in a larger protrusion. An experimental work of Jiang *et al.* also suggested that the local strain near the top end of TSV may be responsible for the protrusion from the observation that a TSV with a higher protrusion is subjected to a higher strain near the top end [23].

4 The general picture of TSV protrusion

For a given blind TSV sample, to predict its protrusion behavior, the loading condition as well as the microstructure should be considered. First, the loading condition should be examined. The most important factor to produce protrusion is a compressive strain ϵ_x or a tensile strain ϵ_y applied near the top end of the TSV. Under the compressive strain ϵ_x , the TSV generally protrude at both edges, with little protrusion occurring in the middle of the top surface. The application of the tensile strain ϵ_y can increase the protrusion height, e.g., a higher protrusion in the middle of the top surface in particular. In addition, the application of shear strain γ_{xy} can lead to a higher protrusion, e.g., the loading condition of $\theta = 150^\circ$ leads to the maximum protrusion from our simulation results. If the applied loading produces protrusion, the microstructure in the TSV needs to be carefully considered. The grains in the top layer contribute more to the protrusion than the grains below. Different grain structures lead to different levels of protrusion height: a smaller grain size along the y -direction, a larger misorientation between the grains and a symmetrical grain structure lead to a higher protrusion.

From the simulation data, a quantitative model to predict

Table 1: The loading distributions in different regions

	Strain rate applied in different regions		
Model No.	$600 \geq y \geq 350$	$350 \geq y \geq 130$	$130 \geq y \geq 0$
M1	1×10^{-4}	5×10^{-4}	10×10^{-4}
M2	10×10^{-4}	5×10^{-4}	1×10^{-4}
M3	10×10^{-4}	5×10^{-4}	10×10^{-4}
M4	5×10^{-4}	10×10^{-4}	5×10^{-4}

Fig. 12: TSVs with different distributions of loading along the edges. The models are (a) M1, (b) M2, (c) M3, and (d) M4 summarized in Table 1. The arrows indicate the loading in different regions. The black dashed curves sketch the protrusion profile.

the protrusion height can be established:

$$h = \sqrt{h_1 + A \cdot \epsilon_x + B \cdot \epsilon_y + C \cdot \gamma_{xy}} \times \sqrt{h_2 + \left(\frac{D}{d} + E \cdot \eta\right) \cdot e^{-F/T}} \quad (5)$$

Fig. 13: The plot of protrusion height versus grain size d and misorientation η . The scattered dots are simulation data and the prediction surface is the result of optimization of the data according to Equation (5).

where h_1, h_2, A, B, C, D, E and F are the parameters needed to be determined. d is the grain size, η is the misorientation between the grains, and T is the temperature. Noted that multiplication is used to connect the two parts in Equation (5), which means that protrusion is only produced when a "right" loading is applied. A set of parameters of $(h_1, h_2, A, B, C, D, E, F) = (1.6, -4.1, 80, 2.2 \times 10^2, 2.2 \times 10^2, 78, 5.9 \times 10^{-2}, 5.2 \times 10^2)$ is determined by an optimization process of the simulation data with respect to Equation (5). Fig. 13 plots the surface of protrusion height versus the grain size d and misorientation η .

A different viewpoint from plastic flow [31] to understand the protrusion behavior of TSVs is proposed to provide a visual guide. By connecting the initial and final positions of the atoms, the flow field can be plotted as shown in Figs. 14b and 14d. A "disordered" region in the flow field is marked out by the dotted ellipse in Fig. 14d. Heterogeneous local deformation occurs in the "disordered" region by the means of GB migration or dislocation motion. With the applied loading $\theta = 150^\circ$, the flow field can be decomposed into two components: one component moves the atoms upwards/downwards and leads to protrusion/intrusion, and the other component rotates the atoms and results in local defor-

Fig. 14: A different viewpoint from plastic flow provides a visual guide of TSV protrusion behavior. (a) and (c): The protrusion/intrusion of TSVs with different grain structures. (b) and (d): The corresponding flow field of the atoms. The dotted ellipse marks out a "disordered" region of the flow field.

mation. As shown in Figs. 14c-14d, more local deformation produced in the TSV means fewer atoms moving upwards and thus producing a lower protrusion.

5 Conclusions

In this study, a two-mode PFC model is used to investigate the Cu-TSV protrusion under different loading conditions from the atomic scale. Simulation results suggest that the combined effects from both the loading condition and the microstructure of copper grains control the complex behavior of protrusion. The following conclusions can be drawn:

(1) To control the protrusion behavior, both the loading conditions and microstructure need to be considered together. For TSVs with the same grain structure, different loading conditions can lead to different levels of protrusion height and profiles.

(2) Under the compressive strain ϵ_x , the protrusion profile generally bumps up near both edges and remains almost flat in the middle of the top surface. However, the application of the tensile strain ϵ_y can increase the protrusion height, e.g., bumping up in the middle of the top surface. In addition, if the TSV is subjected to both the strain ϵ_x and γ_{xy} , the loading direction of $\theta = 150^\circ$ produces the maximum protrusion.

(3) Under the same applied loading that produces protrusion, the microstructure of copper grains in the TSV controls the protrusion behavior:

- The grains in the top layer contribute more to protrusion than the grains below;
- A smaller grain size along the y-direction leads to a higher level of protrusion. Under the loading direction of $\theta = 150^\circ$, a larger grain size along x-direction results in a higher protrusion. However, a larger grain size along the x-direction produces a lower level of protrusion with the application of ϵ_y ;
- A larger misorientation between the grains in the top layer produces a higher level of protrusion;
- A symmetrical Cu-TSV in terms of geometry and interior grain structure under a symmetrical loading condition produces a higher level of protrusion.

(4) A viewpoint from plastic flow can provide a visual guide to understand the behavior of TSV protrusion: more "disordered" regions in the flow field means fewer atoms or grains diffusing upwards, and thus leading to lower protrusion.

Acknowledgements

The authors acknowledge financial support from the National Natural Science Foundation of China (NSFC) under grant 51832002, the Guangdong Natural Science Foundation under grant 2015A030312011, and the Zhuhai Key Technology Laboratory of Wide Bandgap Semiconductor Power Electronics under grant 20167612042080001. Financial support from Zhuhai Rossini Watch Industry Ltd. is also gratefully acknowledged.

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