Research on TSV Thermal-mechanical Reliability Based on Finite Element Analysis

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***Abstract*—Three-dimensional integrated packaging technology is recognized as the fourth generation packaging technology with the hope of breaking Moore's law. And through silicon via(TSV) technology is the key of three-dimensional packaging technology. In order to study the thermal-mechanical reliability of TSV structure, the finite element method was used to simulate the equivalent stress and deformation of TSV with different TSV size, aspect ratio, pitch and structure. The distribution of equivalent stress and deformation was obtained. The simulation results showed that the increase of TSV size would lead to the increase of equivalent stress and deformation, the aspect ratio of TSV would only affect deformation, and the increase of TSV pitch would lead to the decrease of equivalent stress and the increase of deformation. In addition, TSV filled with parylene was analyzed in this paper. The stress could be effectively released by increasing the size of parylene.**

Keywords—thermal-mechanical reliability; TSV; finite element simulation; equivalent stress; deformation

I. INTRODUCTION

Through silicon via (TSV) technology refers to the fabrication of through micro via on silicon wafers in micro-nano processing, so that the distance between the chip and the chip in the vertical direction is the shortest. TSV is the key technology of three-dimensional packaging technology [1-2]. TSV has significant advantages over other three-dimensional package interconnections such as wire bonding, and can be utilized to manufacture devices that are small, high-density, versatile, wide-bandwidth, and highly reliable [3-4]. TSV is a disruptive technology and is considered to be an effective way to achieve the "Super Molar Law", which is widely used in design and production of mainstream devices in the future [5].

However, in the TSV structure, the coefficient of thermal expansion of silicon is about 2.5×10^{-6} /°C, and the coefficient of thermal expansion of copper is about 17.5×10^{-6}/°C [6]. Thermal-mechanical reliability refers to the ability of micro-electromechanical devices to perform specified functions under specified thermal conditions and within specified time. Due to the large difference in thermal expansion coefficients between silicon and copper, large thermal stresses are generated when process temperatures change [7-9]. The residual stress accumulated in the process and the thermal stress in the structure are superimposed, resulting in swelling of the silicon material and delamination of copper and silicon dioxide [10-11]. The thermal-mechanical reliability problem of TSV structure seriously affects the performance of the chip and limits the marketization process of TSV products. Therefore, many scholars at home and abroad have studied the reliability of TSV structure.

At present, academic research on the thermal-mechanical reliability of TSV structure mainly adopts the method of finite element simulation, and some people have carried out related experiments. J.H.Lau et al. analyzed the effects of different TSV pitch and aspect ratio on the stress and strain of silicon and copper by finite element simulation[12-13]. Choa et al. conducted an experimental study on thermal-mechanical reliability of an 8-layer multilayer TSV. It was found that the diameter of the TSV and the thermal expansion coefficient of the filler material have a significant effect on the thermo-mechanical stress [14]. Yu et al. established a wet-heat stress model to study the Hydrogen-based semi-siloxane based TSV wet stress and thermal stress distribution, and coupled the wet-heat stress to the traditional silicon-based TSV [15]. An et al. established a two-dimensional model of the TSV adapter plate, and gave the stress analysis solution for the case where the through hole is completely filled with copper and partially filled with copper. It can be used to discuss the analysis of the TSV stress [16].

However, at present, the study of TSV size parameters does not fully analyze the stress and deformation on key sections, and does not fully consider the factors of size parameters and filler materials. In addition, there is not any suggestion that can effectively reduce the stress and strain of the TSV structure. Based on the finite element simulation, the effects of TSV size, aspect ratio and pitch on the equivalent stress and deformation were discussed. The relationship between the equivalent stress and deformation of the parylene filled TSV size was further analyzed. The effective thermal-mechanical reliability recommendations had certain guiding significance for TSV reliability design. The full text was divided into 5 sections, and the first section was the introduction. Subsequent chapters were arranged as follows: Section 2 established a finite element model based on reasonable assumptions and set simulation parameters. Section 3 discussed the equivalent stress, deformation distribution and critical path distribution of TSV simulation of different size, aspect ratio, and pitch. Section 4 analyzed the different structures and compares the effects of filling parylene and

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changing the size of the filled parylene on stress and deformation. Section 5 summarized the full text, proposed thermal-mechanical reliability recommendations, and looked ahead to future research.

II. FINITE ELEMENT MODELING AND PARAMETER SETTING

In the actual simulation process, finite element analysis is sometimes difficult due to the complex structure of TSV, especially the obvious difference in scale. In order to facilitate the simulation, we propose the following assumptions: (1) Because the barrier layer and redistribution layer are very thin, the influence on the analysis structure can also be neglected, which is not considered in the simulation; (2) Because silicon and silicon dioxide do not reach the plastic condition temporarily under the thermal stress in the simulation process, only elastic deformation occurs, so it is assumed that only elastic deformation occurs in silicon and silicon dioxide,(3) In order to facilitate simulation, it is assumed that all materials are isotropic in the simulation process, which has little influence on the simulation results. Considering the symmetry of the TSV structure, in order to improve the simulation efficiency, a 1/8 axisymmetric model is used in the simulation process. The simplified model of TSV is shown in Figure1, and the meshing is shown in Figure2. Path A is the line from the center of the TSV to the edge of the upper bottom surface, and path B is the line from the center to the edge of the middle section face.

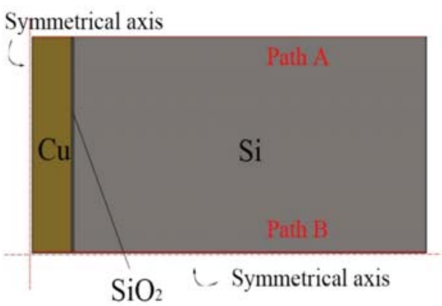
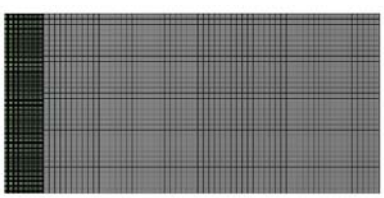


Figure1. TSV simplified model.



(a) Key area meshing

(b) Overall meshing
Figure2. TSV meshing.

In order to study the influence of TSV size and aspect ratio on thermal-mechanical reliability, the TSV pitch is 200μm, the TSV size is changed from 10μm to 40μm, and the aspect ratio is 3, 5, 7, and 10 respectively. In order to study the effect of TSV pitch on thermal-mechanical reliability, when the TSV size is 20μm and the aspect ratio is 5, the TSV pitch varies from 100μm to 400μm for simulation analysis. To investigate the effect of TSV-filled parylene on thermal-mechanical reliability, we considered the simulation of hollow copper columns and parylene filling at a TSV size of 20 μm, an aspect ratio of 5, and a pitch of 200 μm. The size of the parylene in the parylene-filled TSV model is 5 μm, and the size of the hollow in the hollow copper-filled TSV is also 5 μm. In order to study the influence of the size of parylene on the thermal-mechanical reliability, the TSV size is 20μm, the aspect ratio is 5, the pitch is 200μm, and the parylene size is changed from 5μm to 20μm, respectively. The thickness of the silicon dioxide insulating layer between copper and silicon is 0.5 μm. The temperature is ramped from -25 ° C to 125 ° C in the load. The TSV structural material parameters are shown in Table 1.

TABLE I. TSV STRUCTURAL MATERIAL PARAMETERS

Material	Density/($kg{\cdot}m^{-3}$)	Elastic Modulus /GPa	Poisson Ratio
Cu	8900	18.5	0.343
Parylene	1110	6.9	0.35
Si	2334	2.813@25□ 3.107@150□ 3.61@117℃	0.28
SiO2	2400	0.5	0.16

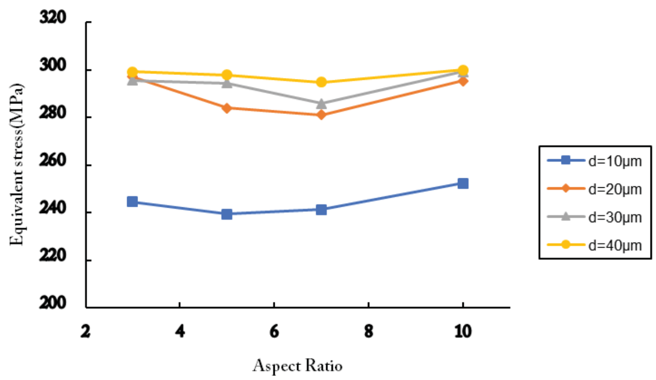
III. ANALYSIS OF SIMULATION RESULTS OF DIFFERENT SIZE PARAMETERS

A. Influence of different TSV size and aspect ratio on the equivalent stress distribution

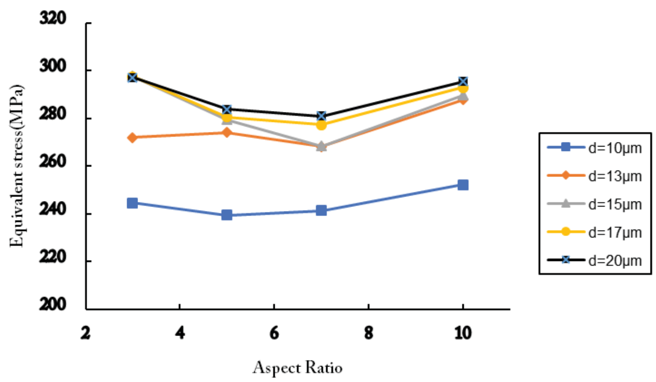
When TSV size is 20μm, the aspect ratio is 5, and the pitch is 200μm, equivalent stress distribution contour is shown in Figure 3. The equivalent stress is mainly concentrated at the interface of copper, silicon dioxide and silicon, and is small on both copper and silicon substrates. Different TSV size and aspect ratio satisfy this law for the equivalent stress distribution contour.

Figure3. TSV equivalent stress distribution contour (deformation magnified 150 times).

Total equivalent stress with different TSV size and aspect ratio is shown in Figure4. It can be seen from Figure 4 that the larger the TSV size, the larger the total equivalent stress, but the increase of the total equivalent stress gradually decreases with the increase of the size. When the TSV size is constant, the aspect ratio of the TSV is changed, and the total equivalent stress variation is small. Therefore, adjusting the TSV size is the main way to change the total equivalent stress of the TSV structure.



(a) Total Equivalent Stress of 10 μm -40μm TSV Size and Aspect Ratio.



(b) Total Equivalent Stress of 10μm -20μm TSV Size and Aspect Ratio..
Figure4. Total equivalent stress with different TSV size and aspect ratio.

When the TSV aspect ratio is 5, the equivalent stress with different TSV size on path A is shown in Figure 5. It can be seen from Figure 5 that on the upper bottom surface, the equivalent stress in the copper-filled TSV structure tends to decrease slightly as the distance from the center increases. The equivalent stress at the interface of the copper, silicon dioxide, and silicon substrate jumps to the highest, and thereafter the equivalent stress on the silicon substrate gradually decreases as the distance from the center increases. The larger the TSV size is, the greater the equivalent stress in each part of the upper bottom surface is.

When the TSV aspect ratio is 5, the equivalent stress with different TSV size on path B is as shown in Figure6. It can be seen from Figure 6 that in the middle section face, the equivalent stress in the copper-filled TSV structure hardly changes, and the variation of the center distance and the TSV size does not affect the equivalent stress, and the rest of the equivalent stress distribution similar to the upper base. The larger the TSV size, the greater the equivalent stress at the interface between copper and silicon, and the greater the equivalent stress on the silicon substrate.

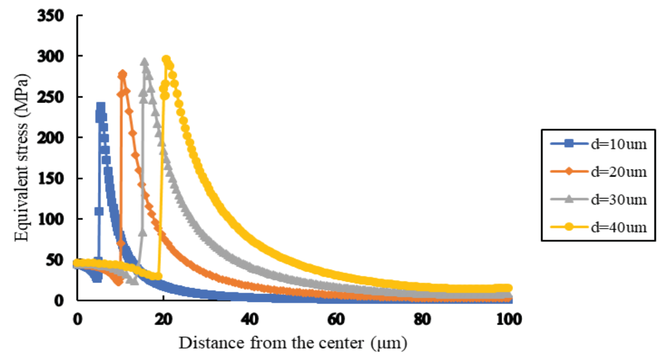


Figure5. Equivalent stress with different TSV size on path A.

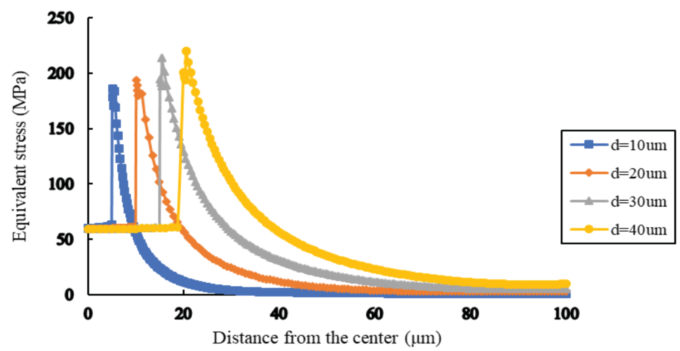


Figure 6. Equivalent stress with different TSV size on path B.

When the TSV size is 20μm, the equivalent stress with different aspect ratio on path A is shown in Figure 7. It can be seen from Figure 7 that on the upper bottom surface, the images of different aspect ratio almost coincide, and the equivalent stress is not affected by the aspect ratio.

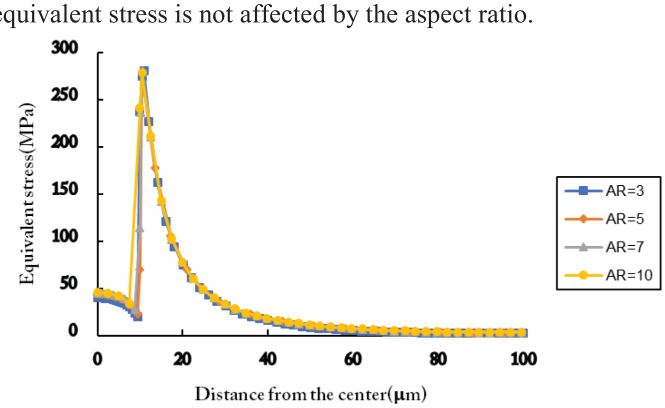


Figure 7. Equivalent stress with different aspect ratio on path A.

When the TSV size is 20μm, the equivalent stress with different aspect ratio on path B is shown in Figure 8. It can be seen from Figure8 that in the middle section face, when the TSVs have the same size and the aspect ratio of the TSV is not less than 5, the equivalent stress on the path A are hardly affected by the aspect ratio. When the aspect ratio of the TSV is less than 5, the equivalent stress is low in the copper-filled TSV.

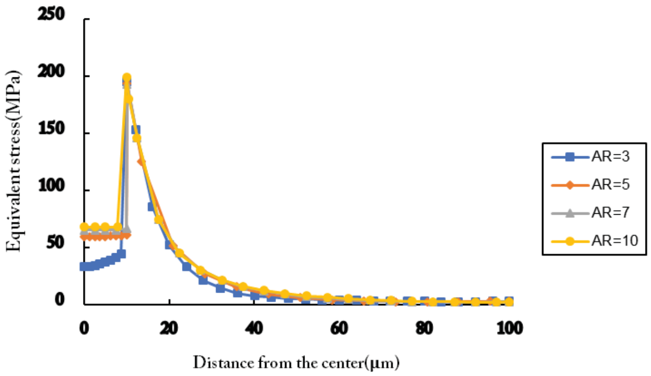


Figure 8. Equivalent stress with different aspect ratio on path B.

B. Influence of different TSV size and aspect ratio on deformation distribution

When TSV size is 20μm, the aspect ratio is 5, and the pitch is 200μm, TSV deformation distribution contour is shown in Figure 9. The deformation is larger on the copper-filled TSV, especially at the copper at the top of the TSV, and the smaller the deformation is toward the inside of the TSV. On the silicon substrate, except for the deformation of the contact with the silica, the deformation of the other portion increases as the center distance increases. Different TSV size and aspect ratio satisfy this law for deformation distribution.

Figure9. TSV deformation distribution contour (deformation magnified 150 times).

The total deformation with different TSV size and aspect ratio is shown in Figure10. It can be seen from Figure 10 that the larger the TSV size, the larger the total deformation; the larger the aspect ratio of the TSV, the larger the total deformation. Under the same TSV size, the aspect ratio of TSV has a certain linear relationship with the total deformation. The larger the TSV size, the greater the rate of change of total deformation. Adjusting the TSV size and aspect ratio can change the overall deformation of the TSV structure.

When the TSV aspect ratio is 5, the deformation with different TSV size on path A is as shown in Figure 11. It can be seen from Figure 11 that in the upper bottom surface, when the TSV size is larger than 10 μm, the maximum value of the deformation is at the center of the upper bottom surface, and thereafter the deformation is reduced as the distance from the center increases. At the interface of copper, silicon dioxide and silicon substrates, the deformation increases slightly with the distance from the center. When the TSV size is less than 10 μm, the maximum value of the deformation is not at the center of the upper bottom surface, but at the edge of the silicon substrate.

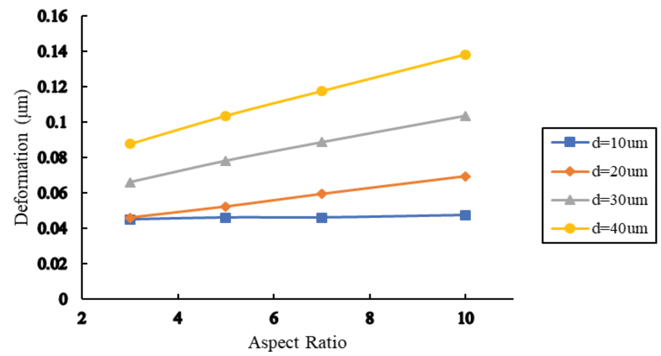


Figure10. Total deformation with different TSV size and aspect ratio.

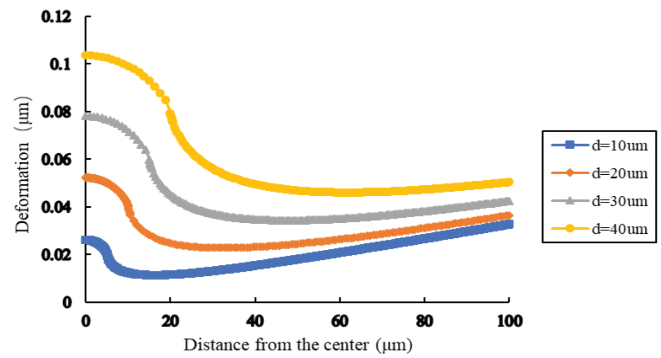


Figure 11. Deformation with different TSV size on path A.

When the TSV aspect ratio is 5, the deformation with different TSV size on path B is as shown in Figure 12. It can be seen from Figure 12 that the equivalent stress gradually increases with the increase of the center distance in the copper-filled TSV structure, reaching a maximum at the interface between copper and silicon, and thereafter the deformation continue to rise after a small decrease and reach a maximum at the edge of the silicon substrate. The larger the TSV size, the greater the deformation at the copper-silicon interface and the greater the deformation on the silicon substrate.

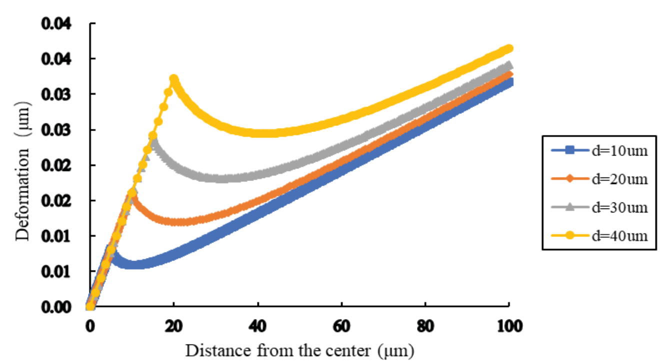


Figure 12. Deformation with different TSV size on path B.

When the TSV size is 20μm, the deformation with different aspect ratio on path A is as shown in Figure 13. It can be seen from Figure 13 that the shape of the deformation curves of the different aspect ratio is similar when the TSVs are the same size on the upper bottom surface. The larger the aspect ratio, the larger the deformation.

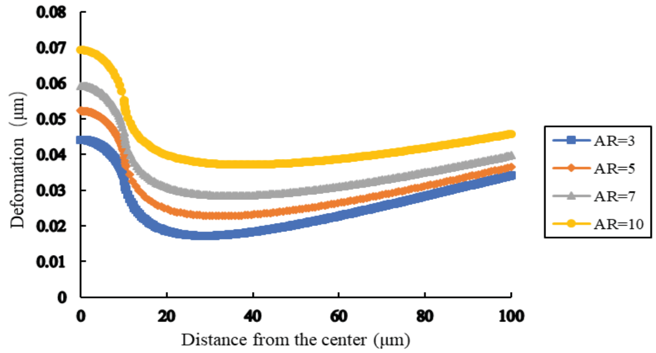


Figure 13. Deformation with different aspect ratio on path A.

When the TSV size is 20μm, the deformation with different aspect ratio on path B is as shown in Figure 14. It can be seen from Figure 14 that when the TSV has the same size and the aspect ratio of the TSV is not less than 5, the deformation is hardly affected by the aspect ratio.

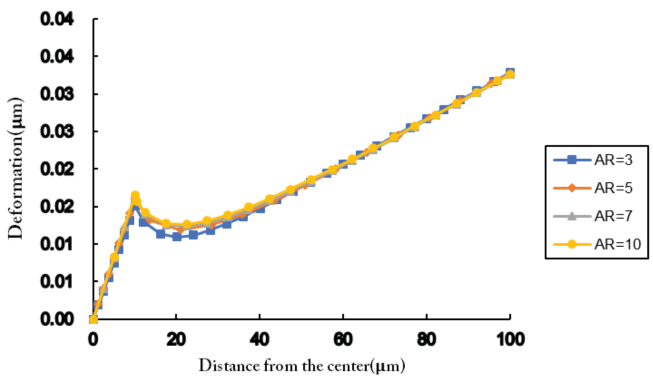
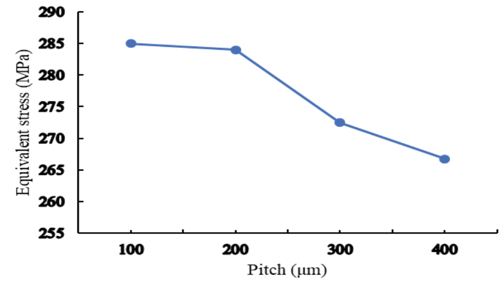


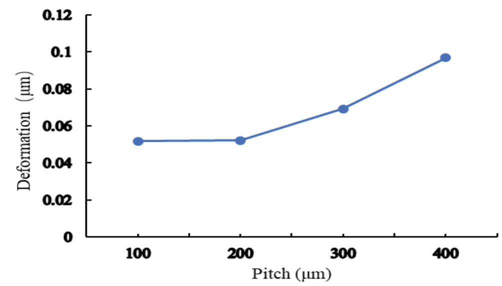
Figure 14. Deformation with different aspect ratio on path B.

C. *Influence of different TSV pitches of equivalent stress and deformation*

When the TSV size is 20μm and the aspect ratio is 5, the different TSV pitch of 100μm to 400μm are taken respectively, and the total equivalent stress and total deformation are shown in Figure 15. It can be seen that as the size and aspect ratio are constant, as TSV pitch increases, the total equivalent stress of the TSV structure decreases and the total deformation increases. When the TSV pitch is greater than 200μm, the influence of TSV pitch on total equivalent stress and total deformation is obvious.



(a) Total equivalent stress with different TSV pitch.



(b) Total deformation with different TSV pitch.

Figure 15. Total equivalent stress and total deformation with different TSV pitch.

IV. Analysis of TSV Simulation Results of Different Structures

A. *Analysis of different filled TSV simulation results*

Total equivalent stress and total strain of different filled TSVs are shown in Table 2. It can be seen that the total equivalent stress of the TSV filled with parylene is smaller than the total equivalent stress of the copper-filled TSV structure, and the parylene-filled structure has certain advantages in thermal-mechanical reliability. The total deformation of the parylene and hollow copper filled TSV is slightly reduced relative to the copper filled TSV.

TABLE II Total Equivalent Stress and Total Strain of TSVs with Different Structures

TSV material	Total Equivalent Stress/MPa	Total Deformation/μm
Copper filled TSV	283.98	0.52252
Parylene Filled TSV	269.15	0.51898
Hollow copper filled TSV	310.89	0.51368

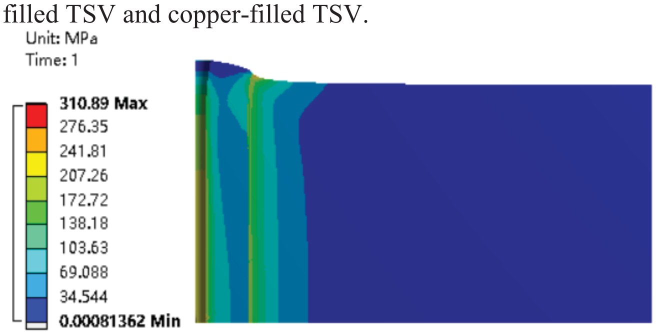
The parylene-filled TSV equivalent stress distribution contour and deformation contour are shown in Figure 16. The equivalent stress increases significantly at the interface between parylene and copper at the interface with copper, silicon dioxide and silicon substrates. The deformation is similar to the copper-filled control group. There is a maximum at the center of the bottom surface of the TSV. On the silicon substrate, except for the deformation at the contact with the silicon dioxide, the deformation of the other part increases as the center distance increases.

(a)Parylene equivalent TSV-filled stress distribution contour.

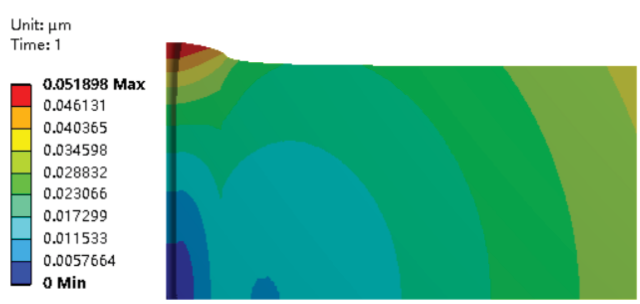
(b)Parylene equivalent TSV-filled deformation distribution contour.

Figure16. Parylene equivalent TSV-filled stress distribution contour, deformation distribution contour (deformation magnified 150 times).

The hollow copper pillar filled TSV equivalent stress distribution contour and deformation distribution contour are shown in Figure 17. The equivalent stress is the highest on the inner side of the hollow copper column, and the junction of copper, silicon dioxide and silicon substrate is obviously higher, and the equivalent stress is the lowest at the silicon substrate away from the center. The deformation of the TSV filled with hollow copper pillars is similar to that of parylene-filled TSV and copper-filled TSV.



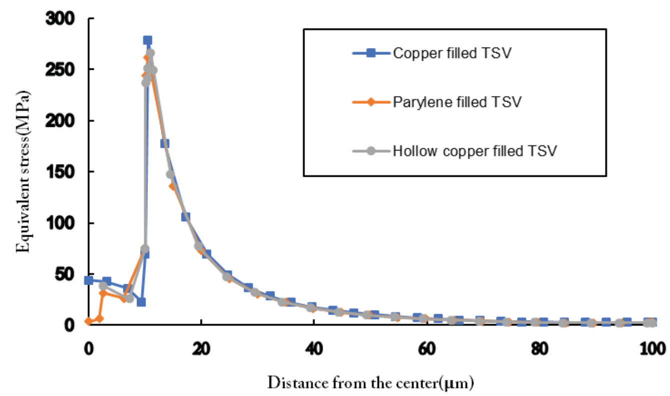
(a) Hollow copper filled TSV equivalent stress distribution contour.



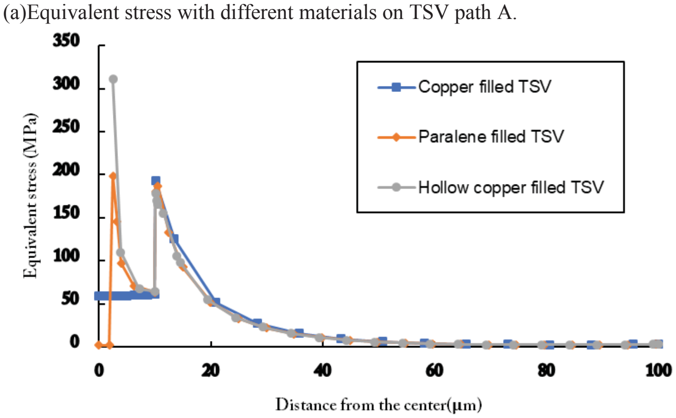
(b)Hollow copper filled TSV equivalent deformation distribution contour.

Figure 17. Hollow copper filled TSV equivalent stress distribution contour, deformation distribution contour (deformation magnified 150 times).

The equivalent stress with different materials on TSV path A and B is shown in Figure 18. It can be seen that on the upper bottom surface, the equivalent stress peak of TSV is at the junction of copper, silicon dioxide and silicon substrate, and the maximum equivalent stress of copper-filled TSV is the largest, and the hollow copper is filled with TSV, and parylene is the second. The fill TSV is minimal. This is because the coefficient of thermal expansion of parylene is less than the coefficient of thermal expansion of copper and acts as a stress release. On path B, the equivalent stress is smaller than the upper surface, and the equivalent stress of the hollow copper-filled TSV on the innermost side of the ring is as high as 310.89 MPa, which is noteworthy.



(a)Equivalent stress with different materials on TSV path A.

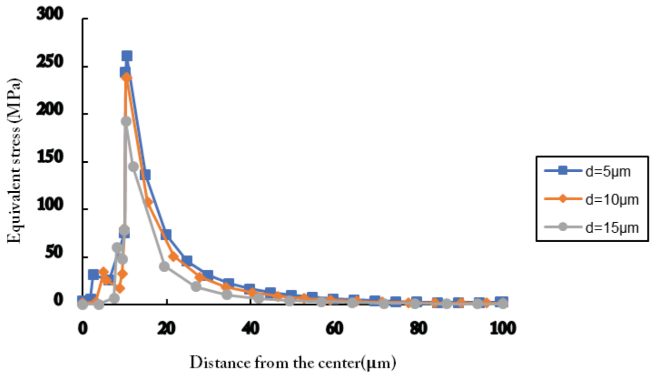


(b)Equivalent stress with different materials on TSV path B.

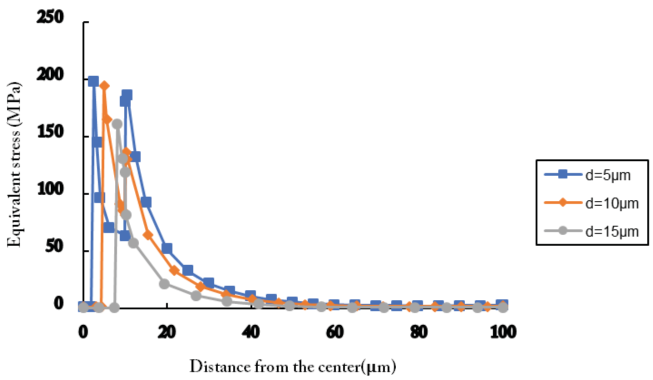
Figure 18 Equivalent stress with different materials on TSV path A and B.

B. Analysis of simulation results of different size of parylene TSV

The equivalent stress with the different size of parylene TSV path A and B is shown in Figure 19. It can be seen that on the upper bottom surface, the equivalent stress peak of TSV is at the junction of copper, silicon dioxide and silicon substrate, and the larger the parylene size, the smaller the equivalent stress of TSV. When TSV size, aspect ratio, and pitch are determined, larger size parylene fill can be considered to improve TSV thermal-mechanical reliability.



(a)Equivalent stress with different size of parylene TSV on path A.



(b) Equivalent stress with different size of parylene TSV on path B.
Figure 19. Equivalent stress with different size of parylene TSV on path A and B.

V. CONCLUSIONS AND PROSPECTS

In this paper, the effects of TSV size, aspect ratio, pitch and structure on TSV equivalent stress and deformation were discussed by using finite element simulation. The conclusions are as follows:

(1) When the TSV aspect ratio is constant, the larger the TSV size, the larger the total equivalent stress and the larger the total deformation. When the TSV size is constant, the TSV aspect ratio is larger, the total deformation is larger, and the total equivalent stress is No significant changes.

(2) The TSV size has a significant effect on the equivalent stress and deformation on the path A, but when the aspect ratio of the TSV exceeds 5, the stress and deformation are hardly affected by the aspect ratio.

(3) After the size and aspect ratio are given, the pitch of the TSV is increased, the total equivalent stress of the TSV structure is reduced, and the total deformation is increased.

(4) Parylene filled TSV can effectively reduce the equivalent stress, and the larger the size of parylene, the more obvious the effect, and the larger size parylene filling can be considered to improve the thermal-mechanical reliability of TSV.

The conclusions obtained in this paper have certain guiding significance for improving the thermal-mechanical reliability of TSV. However, this study still has shortcomings. On the one hand, only the equivalent stress was analyzed, and the radial stress, axial stress and shear stress which constitute the equivalent stress were not separately studied; on the other hand, the research on parylene was not deep enough, only the size is considered. For the case of 20μm, aspect ratio of 5, and pitch of 200μm TSV, there was a lack of comprehensive analysis of the equivalent stress and deformation of parylene size parameters for a variety of different TSV size parameters. The next step is to separately analyze the radial stress, axial stress and shear stress, and discuss the thermal-mechanical reliability of parylene filling under different TSV size parameters.

ACKNOWLEDGEMENT

The research in this paper was funded by the Pre-Research Foundation of National Ministry (Grant No. 41402010401).

The research in this paper was funded by the Project of National Natural Science Foundation of China （Approval No. 51875570）.

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