Thermo-mechanical Simulations of an Open Tungsten TSV

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Abstract

A specific open Through Silicon Via (TSV) technology is analyzed by means of thermo-mechanical Finite Element Method (FEM) simulations in order to assess stress behavior and to identify critical stress points in the structure. An analytical expression is introduced for the stress field around one TSV and its application in the description of the stress in a particular arrangement of vias is discussed. The analysis provides a consistent justification for the robustness of the technology, while it also points out the potential failure points.

Introduction

Three-dimensional (3D) integration in semiconductor technology provides an alternative for keeping the current pace of miniaturization and enhancing devices' capabilities. The advantages can be summarized briefly as increased density, broader functionality, and higher performance per unit area, by making efficient use of the third dimension [1]. However, 3D integration opens up a new myriad of challenges in design and fabrication, which must be overcome in order to achieve large scale production [1], [2].

There are several ways for implementing 3D integration, where a significant number involves an interconnection through silicon with a so-called Through Silicon Via (TSV) to bind the different device layers [2]. One issue with TSVs is the mechanical stability regarding temperature changes in the structure, which is the typical scenario during processing with thermal cycles and also in normal device operation. Our work addresses this problem for a state of the art open TSV (unfilled) technology with the goal to identify potential failures and to acquire advanced insight towards mechanical reliability.

Elastic thermo-mechanical simulations of this TSV technology were performed to accomplish our objective to address not only to the impact of temperature variation in a single TSV, but also to a specific disposition of TSVs in the device. This analysis enables to identify critical points for the TSV itself as well as how the placement of the vias positively influences the reliability of this technology.

Problem description

This work is based on a 3D integration structure which uses wafer bonding and TSVs to directly integrate low output sensors with their associated analog amplification and signal processing circuitry. A diagram of the TSV structure is presented in Fig.1. Metallization and SiO_2 passivation are deposited conformally on the TSV surfaces following the Si etch process. More processing details can be found in [3]. Typical TSV Si etch dimensions are 250µm and 100µm, for depth and radius, respectively. The oxide layer have thickness of 1.0µm and the tungsten layer a thickness of approximately 0.2µm on the TSV wall in the direction towards the silicon.

The most remarkable characteristic of this technology is the usage of an open TSV. This approach has the advantage of reducing the stress impact due to the thermal coefficient (CTE) mismatch between the silicon and the metal, in comparison with the large majority of recently published TSV designs which apply vias filled with some metal, usually copper. Furthermore, the utilization of tungsten as the conductive metal instead of copper reduces the CTE with the silicon and therefore the stress produced by temperature variations.

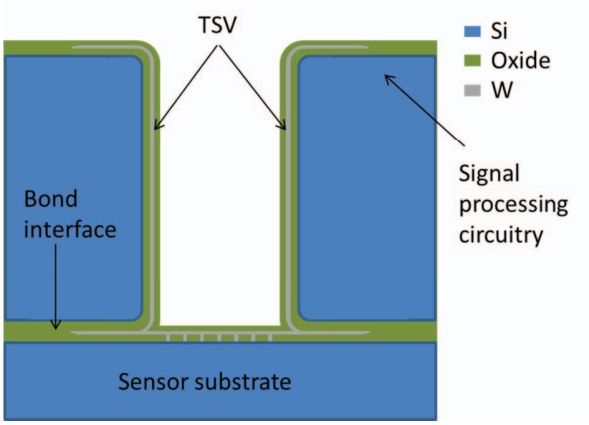

Fig.1 - Schematic overview of our 3D integrated technology using wafer bonding and TSVs.

The TSV's are organized in a particular fashion over the sample as shown in Fig.2. This geometry has an impact on the stress development along the structure, which will be discussed later.

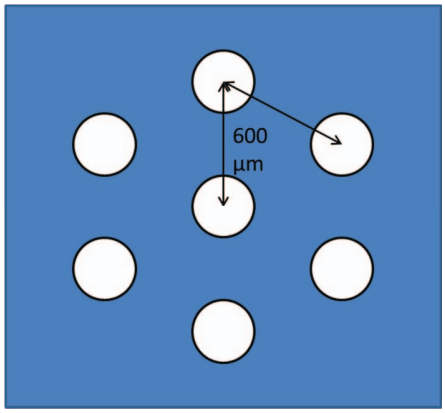

Fig.2 – Top view of the device with the arrangement of 7 TSVs.

During operation the device is expected to work properly in the temperature range of -40ºC to 125ºC. Our main goal is to assess the mechanical response of the structure in this scenario considering the stress free temperature of 25ºC, although, the existence of residual stress in the metal layer of the TSV is known [4]. Furthermore, pre-stress in elastic simulations would only bias the final stress without major modifications to the general behavior. We have not assumed any plasticity effects, because the geometry and the thickness of the layers prevent those to occur.

Simulation setup

As a mean to understand the stress behavior in the TSV structure under the aforementioned conditions, FEM simulations were carried out. Three-dimensional (3D) and two-dimensional (2D) simulations were applied for studying a single isolated TSV. For the constellation of 7 TSVs the 3D simulations were not performed due to the prohibitively large amount of required computational resources to approach properly a problem of this size, therefore only 2D simulations were performed.

The thin layers of tungsten and oxide make the meshing process a challenging task. In order to have a good approximation of the solution in those layers and in the regions surrounding them a very fine mesh is needed. Fig.3 shows the used mesh for the 2D case.

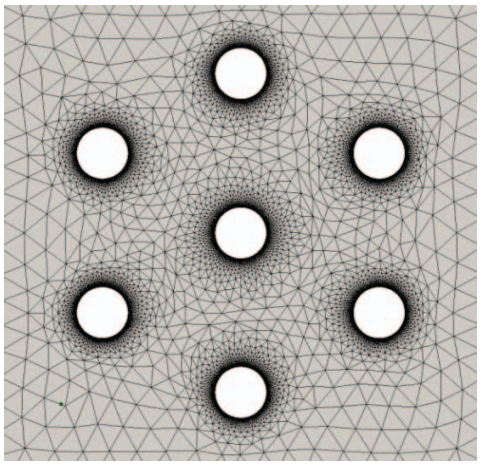

Fig.3 – 2D mesh

For the 3D case we can take advantage of the cylindrical symmetry of the structure to reduce the size of the problem and speed up the meshing process and the simulation itself. In that way only one-quarter of the structure is used. The mesh is presented on Fig.4.

The resulting meshes have 5939 points for the 2D configuration with one single TSV, 49231 points for 2D with the set of 7 TSVs, and 1054616 points for the 3D TSV. Considering linear basis functions for the FEM, it leads to the number of unknowns of 11854, 98302, and 3131322, respectively for each configuration. These numbers document how demanding a simulation with a full set of 7 TSV's in 3D could be.

For the simulations we used our inhouse FEM tool entitled ViennaFEM [5]. It is C++ library based, built under the generic program paradigm, with symbolic computation capabilities. Linear basis functions were used for the solution approximation and the BicGStab method for the linear solver. Pre-conditioning is needed for reliably obtaining results, especially for the 3D case, since the difference between the thin layers and the rest of the structure leads to scaling issues on the linear system. It is also possible to approach this problem by reducing the local meshing growth rate, but this would increase the size of the linear system and slow down the simulation.

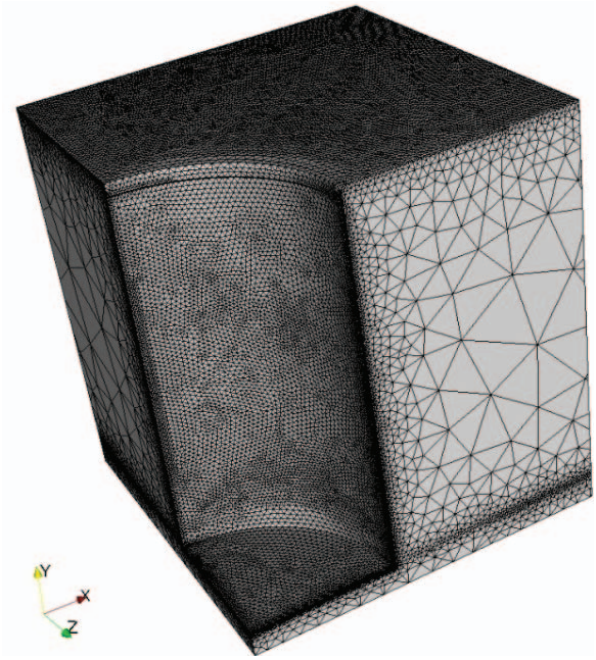

Fig.4 – 3D mesh

A plane-strain approximation was assumed for the 2D simulations, hence the results are only valid for bulk Si in the middle of the TSV, and do not consider the stress at the Si surface (where the CMOS devices are fabricated). Regarding the boundary conditions the square's border is mechanically constrained, while the circle boundaries are free. For the 3D case vanishing displacement at the far sides of the Si body was assumed, however, the top and the bottom of the structure are free to dislocate. Symmetric boundary conditions are imposed on the near side of the domain (x = 0 and z = 0). Concerning material parameters the values from Table I were used.

Table I - Materials constants

Material	Young's Modulus (GPa)	Poisson's ratio	CTE ($10^{-6}K^{-1}$)
Silicon	131	0.27	4.6
Silicon Oxide	72	0.17	0.6
Tungsten	400	0.28	4.4

Results and discussions

First, the 2D simulations were carried out with one single and isolated TSV. Our objective is to understand the stress evolution of one via without any external disturbance of the neighboring TSVs. The resulted stress tensor and Von Mises stress in Cartesian coordinates are depicted in Fig.5.

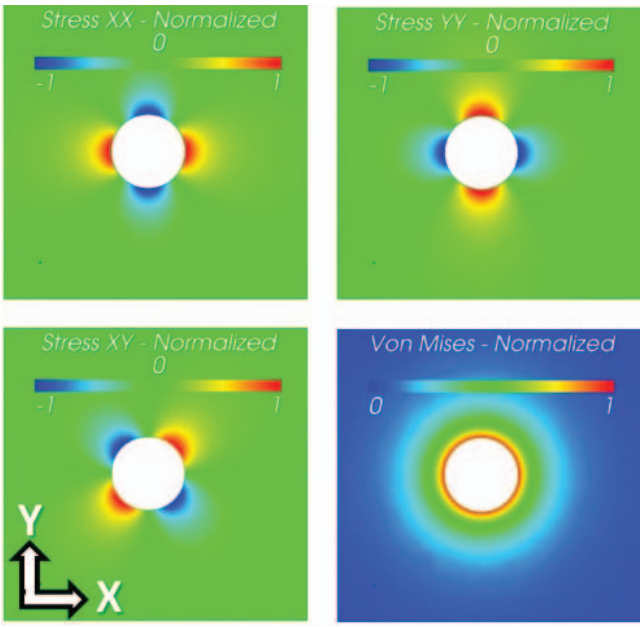

Fig.5 – Stress tensor and Von Mises stress.

As expected, cylindrical symmetry is given in the structure. The stress peak is detected on the tungsten layer and it decays in the direction towards the silicon as shown in Fig.6.

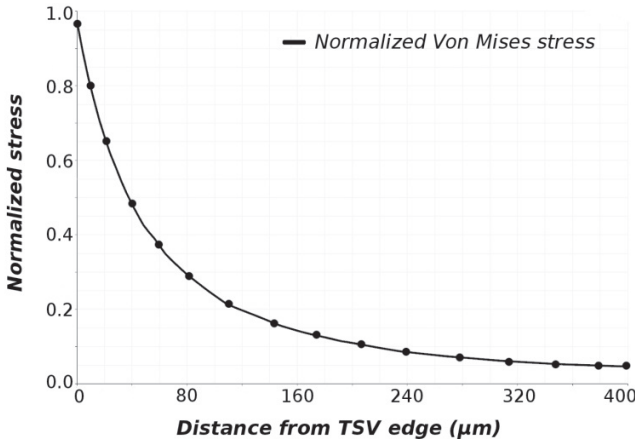

Fig.6 – Von Mises stress towards Silicon.

A previous work [6] has developed an analytical solution for this situation in filled TSVs, which cannot be applied in our case. However, it is still possible to obtain the exact solution for the unfilled TSV problem. For doing so it is necessary to consider the equilibrium equation in cylindrical coordinates as in (1.a) and Hooke's Law with a thermal expansion term as stated in (1.b) [7].

$$\frac{d\sigma_{rr}}{dr} + \frac{1}{r}(\sigma_{rr} - \sigma_{\theta\theta}) = -F \qquad (1.a)$$

$$\begin{bmatrix}\sigma_{rr}\\ \sigma_{\theta\theta}\\ \sigma_{zz}\end{bmatrix} = K\begin{bmatrix}1-\nu & \nu & \nu\\ \nu & 1-\nu & \nu\\ \nu & \nu & 1-\nu\end{bmatrix}\begin{bmatrix}du/dr\\ u/r\\ \varepsilon_{zz}\end{bmatrix} - \sigma_T\begin{bmatrix}1\\1\\1\end{bmatrix} \qquad (1.b)$$

$$K = \frac{E}{(1+\nu)(1-2\nu)}\ ;\ \sigma_T = \frac{E\alpha\Delta T}{1-\nu}$$

σ and u are the stress tensor and displacement field in cylindrical coordinates, respectively, E is the Young modulus, ν is Poisson ratio, α is the CTE, F is the body force, and ε_{ZZ} is the normal strain in z-direction, which vanishes in the plane-strain approximation. Since no body force is present in the problem, equation *(1.a)* becomes a homogeneous PDE with the solution in the displacement field given by (2).

$$u(r) = Ar + \frac{B}{r} \qquad (2)$$

A and B are integration constants. This solution is valid for every point in the structure, however, the difference among materials is determined by the integration constants which are obtained from the boundary conditions and interface conditions along the domain. A general picture of the solution is shown in Fig.7.

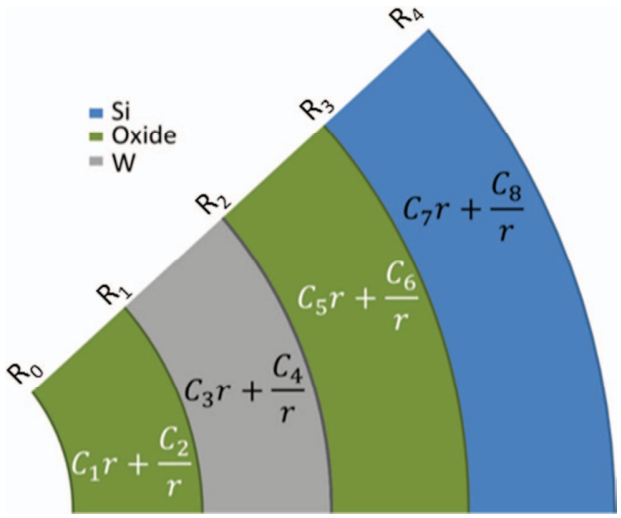

Fig.7 – Solution along the TSV's layers.

C_i are the integration constants of the solutions in each subdomain (material). Applying the boundary conditions described in section "Simulation setup" and enforcing displacement and stress continuity between the material interfaces one can derive a linear system to obtain the integration constants. The system is shown in the set of equations (3).

Displacement continuity

$$C_1R_1 + \frac{C_2}{R_1} = C_3R_1 + \frac{C_4}{R_1}$$
$$C_3R_2 + \frac{C_4}{R_2} = C_5R_2 + \frac{C_6}{R_2} \qquad (3.a)$$
$$C_5R_3 + \frac{C_6}{R_3} = C_7R_3 + \frac{C_8}{R_3}$$

Stress continuity

$$K_{oxide}\left[C_1 + \frac{(2\upsilon-1)C_2}{R_1^2}\right] = K_W\left[C_3 + \frac{(2\upsilon-1)C_4}{R_1^2}\right]$$
$$K_W\left[C_3 + \frac{(2\upsilon-1)C_4}{R_2^2}\right] = K_{oxide}\left[C_5 + \frac{(2\upsilon-1)C_6}{R_2^2}\right] \qquad (3.b)$$
$$K_{oxide}\left[C_5 + \frac{(2\upsilon-1)C_6}{R_3^2}\right] = K_{Si}\left[C_7 + \frac{(2\upsilon-1)C_8}{R_3^2}\right]$$

Boundary conditions

$$\sigma_{rr}(R_0) = K_{oxide}\left[C_1 + \frac{(2\upsilon-1)C_2}{R_0^2}\right] = 0$$
$$u(R_4) = C_7R_4 + \frac{C_8}{R_4} = 0 \qquad (3.c)$$

Although the full development of the analytical solution is feasible, it is very lengthy. A faster approach is to compute the constants directly with a linear solver or with the transfer matrix method.

An additional consideration can be done to simplify the solution. Since the domain's dimensions are far larger than the stress spread zone, it is possible to consider the exact solution under the infinite plane approximation. In that situation the constant value C_7 vanishes and one can calculate the displacement and stress in silicon for the TSV by (4).

$$u_{Si}(r) = \frac{-11.154}{r} \qquad (4.a)$$

$$\sigma_{rr}^{Si} = \frac{E(2\nu-1)}{(1+\nu)(1-2\nu)}\frac{-11.154}{r^2} + \sigma_T \qquad (4.b)$$

$$\sigma_{\theta\theta}^{Si} = \frac{E(1-2\nu)}{(1+\nu)(1-2\nu)}\frac{-11.154}{r^2} + \sigma_T \qquad (4.c)$$

In Fig.8 the displacement evolution in silicon along the radius of the TSV in comparison with the exact solution given in (4.a) is shown.

Additional insight is provided by 3D elastic thermo-mechanical simulation of the isolated TSV. During the thermal cycling, 3D geometrical features influence the distribution of mechanical stress, especially on the top and the bottom of the via. Hence 3D simulations enable the determination of sites, which are particularly exposed to high mechanical stress. Fig.9 shows the Von Mises stress for one quarter of the TSV.

With 2D and 3Dsimulations one can have different but complementary perspectives of the thermal stress development in the structure.

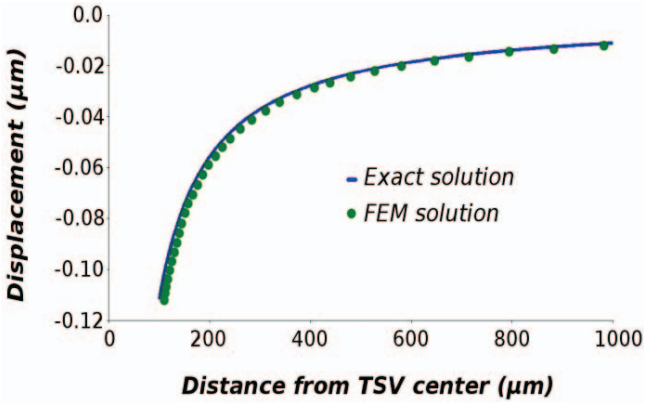

Fig. 8 – Comparison between FEM and exact solution.

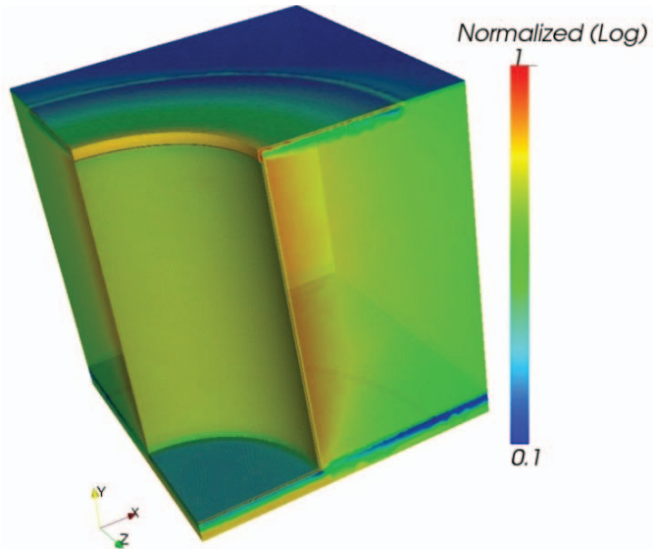

Fig.9 – 3D Von Mises stress in log-scale.

In the 2D case it is possible to observe how quickly the stress drops towards the Si. Due to this fact the region possibly subjected to fatigue (silicon cracking and crack propagation) is very small. In the 3D case one can see that the highest stress is developed in the metal layer at the bottom and near the top of the structure. Here we have a combination of two impact factors: the first is the thermal mismatch between the metal and the surrounding layers and the second is the geometry. High mechanical stress in connection with microstructural properties, which weaken the stability of the crystal (dislocations, grain boundaries), can cause a fracture of the metal layers ending in a complete failure of the TSV.

Although one isolated TSV is not very common in real devices, its analysis is extremely useful in those situations, as can be seen in the following case of the particular arrangement of TSVs as presented on Fig.2.

2D simulations of the 7 TSVs group were performed. The result enables the analysis of the stress field interaction between the TSVs. Fig.10 shows the development of the Von Mises stress. One can notice a peculiar pattern formed in this

structure. Superposition of the individual stress fields of the TSVs leads to stress free regions in between them. Fig.11 details the stress between the two TSVs along the line T1-T2 and it shows the superposition of the stress field of the two vias as described by (4.b).

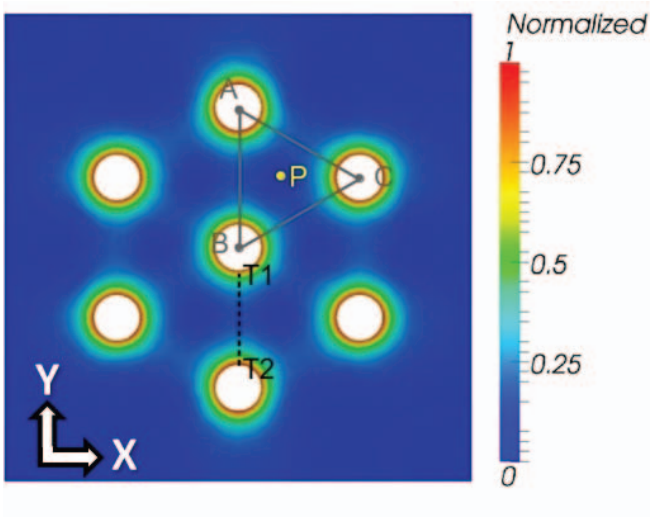

Fig.10 – Von Mises stress for a group of 7 TSVs

Actually, it is possible to use the stress solution for one TSV and the superposition principle to determine the localization of the free-stress zones. We consider the triangle ABC of Fig.10, where the stress inside this triangle is determined only by the TSVs on each of its vertices. The influence of the others TSVs in the arrangement is negligible because of the large distance to the triangle zone. Therefore the localization of the stress minimum value is given by the solution of the problem posed by (5).

$$\min_{r\in\Delta ABC} \sigma^{A}_{Mises} + \sigma^{B}_{Mises} + \sigma^{C}_{Mises} \qquad (5)$$

$$Where, \qquad \sigma_{Mises} = \sqrt{\frac{\sigma_{rr}^2 + (\sigma_{rr} + \sigma_{\theta\theta})^2 + \sigma_{\theta\theta}^2}{2}}$$

The superscript *A*, *B,* and *C* refers to the TSVs on the triangle's vertices of Fig. 10. In this situation, σ_{rr} and $\sigma_{\theta\theta}$ of each TSV is given by (4.b) and (4.c) translated according the origin of the coordinate system used for the minimization problem in the triangle. The point obtained for this particular arrangement is indicated in Fig.10. It is located 170µm in the x-direction and 300µm y-direction away from the center of the TSV in Vertex B.

As a matter of fact this point is the barycenter of the triangle ABC, which in an equilateral triangle is equally far from each vertex, therefore it is the point inside the triangle least influenced by the stress field of the three TSVs. So it is possible to determine the localization of each minimum in this arrangement of TSVs just by the determination of the barycenter of each triangle which composes it. For any other arrangement a new minimization problem must be formulated as it was done in (5).

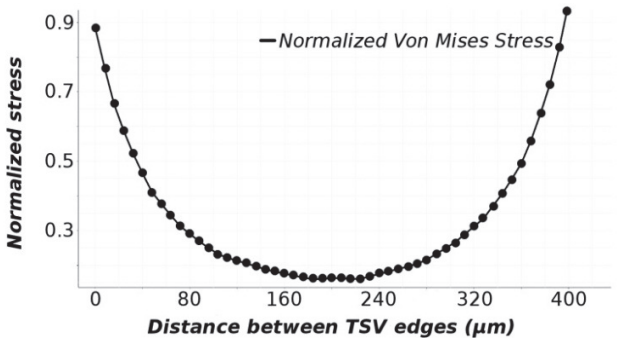

Fig. 11 – Von Mises stress along line T1T2

Summary and Conclusions

In this work a study of the mechanical reliability of an open TSV technology was presented. FEM elastic thermal-mechanical simulations were performed with the purpose to analyze the stress behavior along the via and in the silicon surrounding it.

Critical stress points on the metal layer on the top and bottom of the TSV were identified by means of FEM simulations. It was also shown how the stress develops in the bulk Si, and it was demonstrated that it drops proportionally to the squared distance of the via border.

A method for calculating the exact stress in the middle region of an open TSV was also presented. The results were successfully used to predict the points of minimal stress in the arrangement of TSVs, explaining how the spacing and the constellation of TSVs support high mechanical stability and reliability of the whole structure. The same procedure can be used in others geometries of vias' placement to study the mechanical stability.

Acknowledgments

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