Three-Dimensional Simulation for the Reliability and Electrical Performance of Through-Silicon Vias

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***Abstract*—The electrical performance and reliability of a through-silicon via is investigated through two-dimensional and three-dimensional simulations. Due to the large differences in material thicknesses present in the structures, a 3D simulation is often not feasible. The thermo-mechanical stress, the electrical parameters including TSV resistance and capacitance, as well as the electromigration-induced stress are investigated. A comparison between the results obtained through 2D and 3D simulations is used to suggest which types of simulations require a 3D modelling approach. It is found that an appropriate analysis of the current density through the structure requires 3D simulation, meaning that electromigration phenomena must be studied with 3D simulation or at least a combination of 2D and 3D analysis. However, a 2D simulation with assumed rotational symmetry is sufficient to estimate the thermo-mechanical stress distribution through the structure as well as the parasitic capacitance and signal loss of the TSV.**

I. Introduction

Three-dimensional (3D) integration of integrated circuits (ICs) has become a key challenge for the future evolution of the semiconductor industry. The implementation of a through-silicon via, an essential component for 3D integration, allows for the fabrication of a system connecting several technologies and dense device packing [1]. There are several studies which investigate the reliability and performance of filled copper TSVs [2] as well as open tungsten TSVs. Filled copper TSVs can usually be simulated with 3D models, when the thin Ta/TiN liner material is ignored [3]. Open TSVs are desired, when stress build-up due to material thermal expansion is a concern. The presence of a hole through the TSV gives the metal layer space to expand, avoiding the reliability concerns related to copper pumping [4]. However, in the case of open TSVs, the conductive metal layer is a very thin coating layer which lines the walls of the etched hole. When this layer is present, along with additional thin silicon dioxide and silicon nitride liners, the thickness variation between the different materials becomes very large. Since accurate TSV simulations require a high quality mesh, or at least locallized mesh refinement, a 3D mesh of the full structure is frequently not feasible, and one must resort to 2D simulations with the assumption of rotational symmetry [5].

In this work, a complete 3D mesh of the TSV structure is created using the ViennaMesh toolkit [6] and its sizing framework [7] combined with the TetGen [8] meshing kernel to achieve desired local element sizes, as shown in Fig. 1. Simulations are performed on the 3D structure, as well as on a 2D structure with rotational symmetry, shown in Fig. 2, in order to identify, whether 2D simulations are sufficient when analyzing these types of structures. The electrical performance of the TSVs is analyzed through simulations of the parasitic capacitance, resistance, and frequency-dependent signal loss. Additionally, the thermo-mechanical stress response and electromigration (EM)-induced stress is compared between the two simulation approaches. During the thermo-mechanical simulation, the metal is treated as a linear elastic material with boundary conditions shown in Fig. 2.

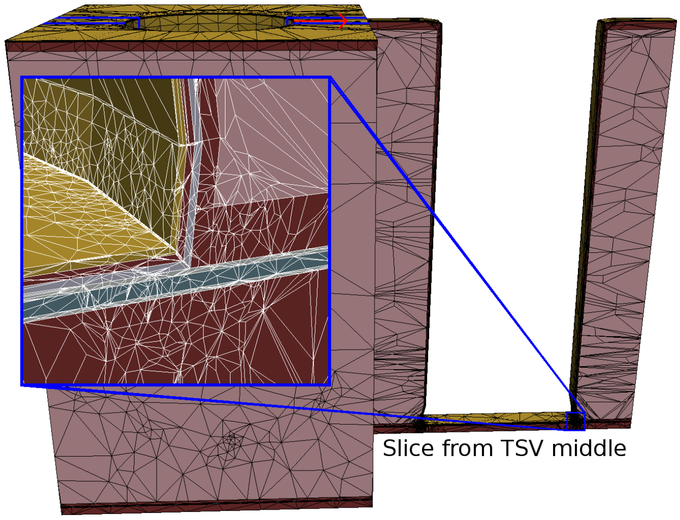

Fig. 1. Full three-dimensional TSV structure with mesh. A thin slice through the TSV middle is shown on the right for a clearer view of the TSV. A zoomed-in section where tungsten and metal meet at the TSV bottom is also shown. A finer mesh is generated at this location in order to enable more accurate simulations of the current density in the area.

II. TSV Structure Generation

Due to the size (80μm$\times$250μm) and complexity of the TSV, a discussion of all required processing steps to fabricate the structure is not included in this work. In particular, the scallops which appear on the TSV sidewalls after etching through the silicon are not considered in the simulations [3]. However, the notching at the TSV bottom is extracted from TEM images and is included in the final test structure [5]. The silicon dioxide layer which separates the bulk silicon from the TSV metal layer is deposited using plasma-enhanced chemical vapor deposition (PECVD) and a sub-atmospheric chemical vapor deposition (SACVD). The models for PECVD and

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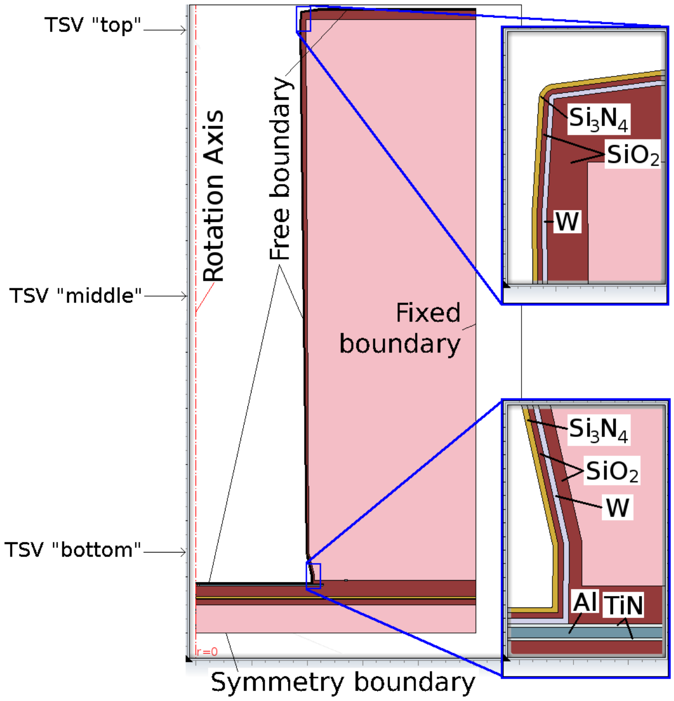

Fig. 2. View of the TSV structure and rotation axis for two-dimensional simulations. The boundary definitions refer to their settings during the thermo-mechanical simulation

SACVD are implemented into the in-house tool DEP3D [9]. The additional thin layers of tungsten (W), oxide (SiO_2), and nitride (Si_3N_4) are deposited on the TSV sidewalls using an isotropic deposition model. The 3D structure used for the 3D simulations is shown in Fig. 1; similarly, the 2D slice of the structure used for simulations which employ rotational symmetry is shown in Fig. 2. The 3D structure is generated using the same models as for the 2D TSV, ensuring that material thicknesses for the 2D and 3D test structures are identical. However, due to the limitations of the representation of cylindrical shapes in a 3D environment, the cylinder is represented as a icosikaitetragonal (24 sides) pillar.

III. TSV Performance

The performance of the TSV is analyzed using simulations of the thermo-mechanical stress generation, TSV electrical performance and paraistics, and EM-induced stress. Simulations using identical models for the 3D and the 2D structure are performed and the results are compared.

A. Thermo-Mechanical Stress Analysis

The thermo-mechanical stress through the TSV structure is investigated by assuming a stress-free temperature of 320°C and cooling the structure down to 20°C. This temperature drop causes the materials to expand or contract, depending on their coefficients of thermal expansion (CTE). For the relevant materials required for the presented TSVs, the CTEs used are listed in Table I, with a linear elastic material model used for the simulation. The resulting stress along one-dimensional cut lines through the structure along the TSV sidewall is shown in Fig. 3, while Fig. 4 shows the stress through the silicon layer, moving away from the TSV hole. The stress generated

TABLE I. Coefficients of thermal expansion for all relevant materials

Material	W	SiO_2	Si	Si_3N_4
CTE (10^{-6}/K)	4.5	0.5	2.6	2.3

at the top, middle, and bottom of the TSV are not identical, with the lowest stress noted through the TSV top. This stress reduction is due to the sides and bottom of the TSV having a fixed/symmetry constraint while the materials at the TSV top have more freedom to expand.

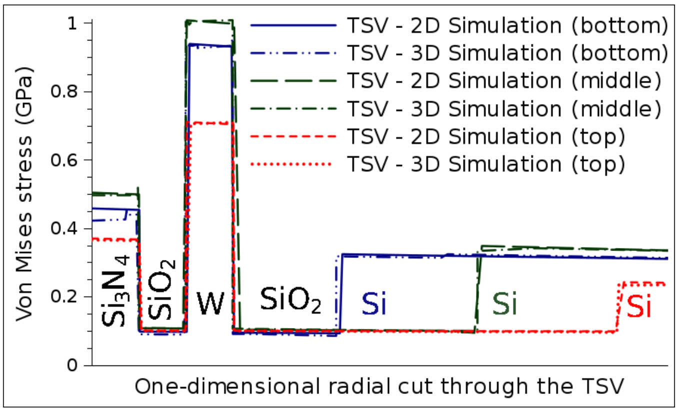

Fig. 3. Thermal stress response (GPa) through the thin liner materials. The thermal simulations are obtained by cooling the structure to a room temperature of 20°C from a stress-free temperature of 320°C.

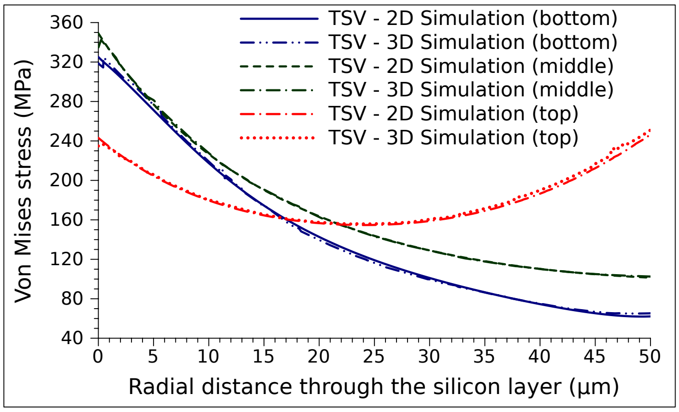

Fig. 4. Thermal stress response (MPa) through the silicon layer. A radial distance of 0μm refers to the oxide/silicon interface. The thermal simulations are obtained by cooling the structure to room temperature 20°C from a stress-free temperature of 320°C.

It can be noted that the simulations which were performed using the 3D structure resulted in a thermal stress identical to those seen using the 2D structure simulation. This is also summarized in Table II, where the average stress at the material interfaces and through the different materials is given for the 2D and the 3D simulations. It should also be noted that, the 3D simulation may vary slightly due to the limitations of representing a cylindrical structure using a finite element mesh.

B. TSV Electrical Performance

The availability of a 3D-meshed TSV enables for the simulation of the current density through the structure with the

TABLE II. THEMO-MECHANICAL STRESS AT MATERIAL INTERFACES AND THROUGH THE MATERIALS PRESENT AT THE TSV SIDEWALL.

Average stress at material interfaces (MPa)		
Interface	**2D & rotation**	**3D simulation**
Si/SiO_2	218	219
SiO_2/W	526	527
W/SiO_2	532	530
SiO_2/Si_3N_4	295	296
Si_3N_4/Ambient	485	485

Average stress through materials (MPa)		
Material	**2D & rotation**	**3D simulation**
Silicon	163	152
SiO_2 insulation	97	97
Tungsten	888	861
SiO_2 liner	92	91
Si_3N_4 liner	422	406

current applied at one side of the TSV, while the 2D simulation assumes a homogeneous current density distribution throughout the structure. This is visible in Fig. 5, where a current of 1A is applied. A 2D slice of the current density through the bottom

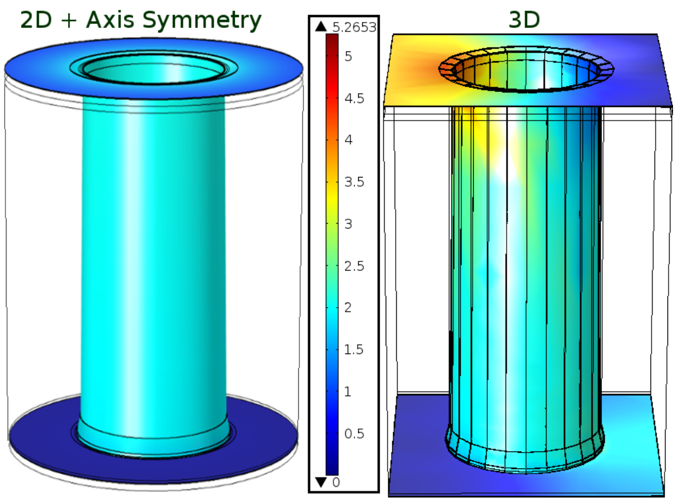

Fig. 5. Three-dimensional view of the current density distribution (MA/cm^2) when the TSV is operating under a 1A current for the (left) two-dimensional simulation and (right) three-dimensional simulation.

of the TSV, where proper mesh refinement is implemented, is shown in Fig. 6. A definite increase in the maximum current density through the structure is evident, when a 3D simulation is performed. This results in an increased effective device resistance by approximately 6.6% and a very slight ($\sim$1%) increase in the low-frequency capacitance, shown in Fig. 7. The increased current density through the aluminum layer suggests that the device is more vulnerable to EM-induced stresses than estimated with 2D simulations.

The frequency-dependent signal loss (S21) for the TSV is shown in Fig. 8 for both structures under test. From the obtained results it can be concluded that a 2D simulation with assumed rotational symmetry is sufficient for analyzing the electrical parameters of open tungsten TSV structures, but when the current density distribution must be known, a 3D model should be used.

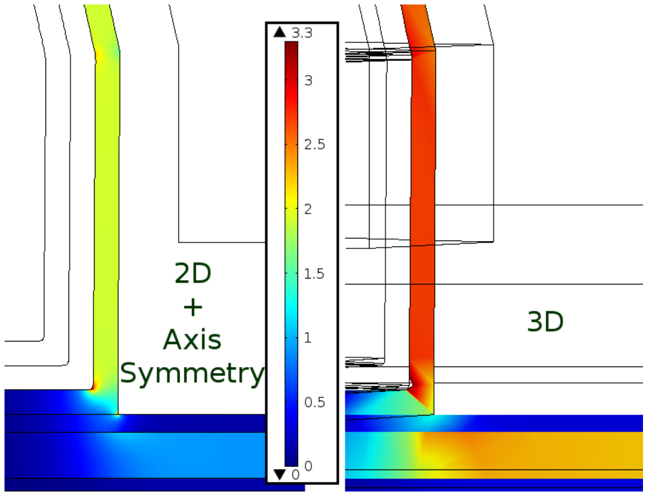

Fig. 6. Two-dimensional view of the current density distribution (MA/cm^2) when a 1A current is applied through a slice of the TSV bottom, where the tungsten and aluminum layers meet. The current density through the 3D structure reaches approximately $2.9MA/cm^2$ while the 2D structure reaches approximately $1.1MA/cm^2$ in the aluminum layer, which is sensitive to electromigration failure.

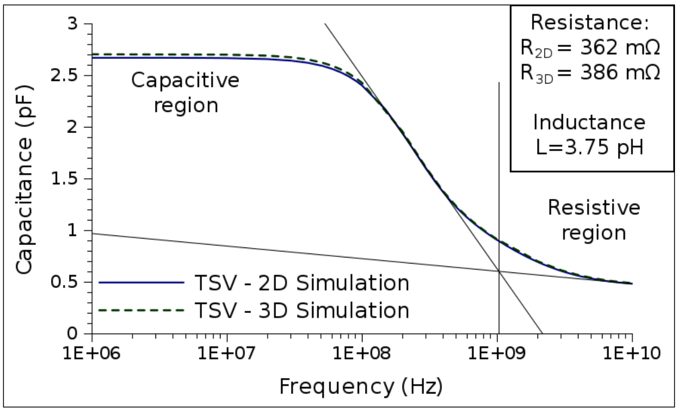

Fig. 7. Frequency dependence on the capacitance through the TSV. The 3D simulations differed in that the terminal where the potential is applied is limited to only one side of the TSV. Due to the axial symmetry in the 2D simulation, the potential is applied from all sides of the structure simultaneously. A slight increase in the resistance for the 3D model is noted (6.6%); otherwise, the results do not show a significant variation.

C. *Electromigration-Induced Stress*

Due to the observed difference in the current density distribution, when a 3D model is used, the EM-induced stress is also expected to experience a significant increase. The EM simulations are performed for an applied current of 1A at a stress-free temperature in order to avoid thermal effects in the TSV. The aluminum, where EM is of highest concern, experiences a maximum current density of about $2.9MA/cm^2$, which is significantly higher than the current density observed with 2D simulations ($1.1MA/cm^2$). Since the current density plays a major role in determining EM-induced stress, this factor must be taken into account when simulating EM. The model used in order to calculate the electromigration-induced stress through the TSV metal layers is given in [10]. The stress is used to detect early failures in metal lines, when compared to a critical stress, which is a material-dependent property.

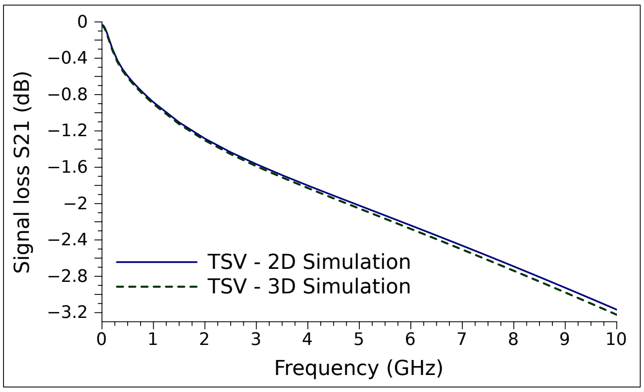

Fig. 8. Frequency dependence on the signal loss (S21 - dB) through the TSV. The 2D simulation with assumed rotational symmetry is sufficient for the analysis.

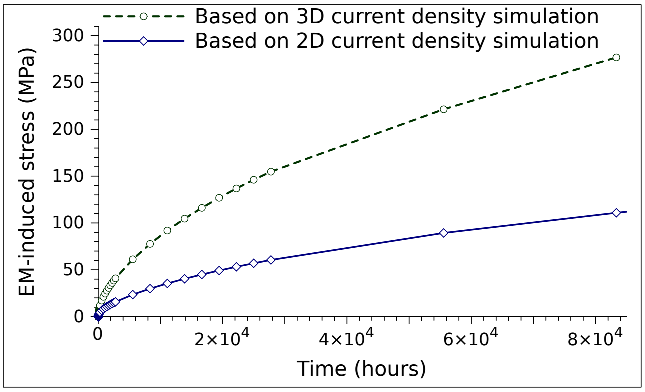

Fig. 9. Maximum electromigration-induced stress in the aluminum layers of the two structures versus time. The current density through the bottom tungsten and aluminum are shown in Fig. 6. The increase in the stress is in line with the increase in the maximum current density through the aluminum.

The evolution of the maximum stress in the aluminum layer of the two structures is plotted in Fig. 9. The effect of the increased current density is immediately evident with the increase in EM-induced stress by a factor of approximately 3. The induced stress at the end of a 10 years period for the two different current density levels is depicted in Fig. 10. When a 2D structure is simulated, a stress level of approximately 100MPa is observed, while a 3D simulation reveals a stress of approximately 330MPa. The 2D simulation assumes this stress distribution around the entire circumference of the TSV, while the 3D simulation mimics realistic operating conditions and enables the potential to be applied from a single side of the TSV. This results in an increased current density distribution on the sides of the TSV, where the potential is applied, which has a direct influence on the vacancy transport and electromigration.

IV. Conclusion

Open TSV structures are frequently fabricated with a deposition of thin layers lining a deeply-etched cylindrical trench. The presence of these layers, which include the conductive TSV metal, often makes the generation of a high-quality 3D mesh unfeasible, or too large to perform complex simulations, such as EM-induced stress computations. Here, a 3D TSV structure is meshed and imported into a finite element tool

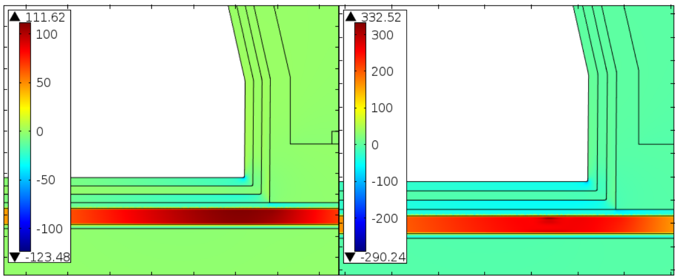

Fig. 10. 2D view of the electromigration-induced stress (MPa) after 10 years of operation. The left and right structures correspond to the current density levels observed in the left (2D) and right (3D) structures shown in Fig. 6, respectively. The maximum stress is observed in the aluminum layer, just below the tungsten lining the TSV sidewalls.

for device analysis. The mesh was successfully generated using the open source tool ViennaMesh [6], and its sizing framework with the TetGen meshing kernel [8].

The results are compared to those of a structure analyzed using a 2D model with rotational symmetry. It was found that the simulated thermo-mechanical stress using the 3D geometry is identical to the one obtained using a 2D geometry. The electrical parameters, such as resistance and capacitance, can also be computed using 2D models with a relatively insignificant error; however, the EM-induced stress requires more accurate information on the current density distribution through the TSV structure. This is only obtainable through 3D simulations and the change in the induced stress, when 3D modeling is applied, is found to be significant enough to conclude that a 2D simulation is not sufficient.

Acknowledgment

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