# Impact of Bosch Scallops Dimensions on Stress of an Open Through Silicon Via Technology

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**Abstract**

The through Silicon Via (TSV) is a lead topic in interconnects and 3D integration research, mainly due to numerous anticipated advantages. However, several challenges must still be overcome if large scale production is to be achieved. In this work, we have studied the effects of Bosch scallops concerning mechanical reliability for a specific TSV technology. The presence of scallops on the TSV wall modifies the stress distribution along the via. By means of Finite Element Method (FEM) simulations, we assess this change in order to better understand the process. The achieved results support experiments and give further insight into the influence of scallops on the stress in an open TSV.

## 1. Introduction

Thermal and intrinsic stresses account for several reliability issues on TSV's. Consequently, they have become a major concern in mechanical stability design [1][2][3]. The thermo-mechanical stress arises from the difference between the coefficient of thermal expansion (CTE) of silicon – which surrounds the via – and the interconnection metal. Meanwhile, the intrinsic stress results from different physical mechanisms which take place during metal deposition.

The impact of each stress can be controlled by the choice of materials and the geometry forming the TSV. A good design should manage the mechanical issues while not comprising the electrical demands of the device. One of the most common and well documented layouts is the cylindrical copper TSV (Fig. 1a). The good electrical properties of copper and the ease of fabrication are an advantage of this technology. However, the difference of more than one order of magnitude between silicon and copper CTEs compromises its mechanical reliability.

CTE mismatch can be compensated with various strategies, for instance by the use of polymer liners around the TSV [4]. The liners work as a barrier which absorbs the stress and hinder its propagation towards the silicon (Fig. 1b). Another approach is the use of an open (unfilled) TSV instead of a filled via [4][5] (Fig. 1c). This scheme reduces the amount of material in the structure and provides room for the metal to expand freely towards the axis of the via leading to an overall stress reduction. Additionally, the stress induced by the TSVs in the silicon can be attenuated by their particular placement [5]. A device usually has several vias close to each other, which can be arranged in such a way so that stress is mutually cancelled or reduced among them.

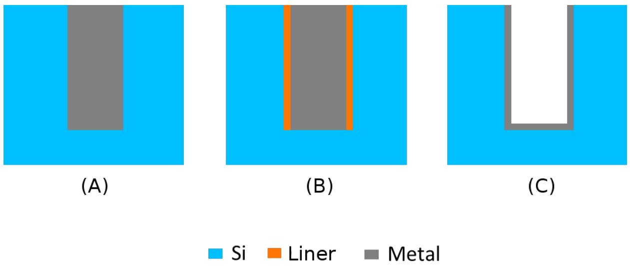


Figure 1. Three cylindrical TSV designs: Filled (A), filled with liners (B), and open (C).

A 3D integration technology was recently introduced based on an open TSV [6], and since then several papers have been published about its mechanical [5][6][7] and electrical properties [8]. So far, the structure has proved itself to be reliable and mechanical stable, but a recent paper of Krauss et al. [7] reported an uncommon behavior of the stress in the via. Krauss et al. performed mechanical characterization of the structure and learned that the intrinsic stress inside TSV's metal layers was four times smaller than expected. This phenomenon was not entirely understood, although Krauss et al. has identified Bosch scallops – created during open TSVs processing – as a possible cause. We tested Krauss hypothesis by means of Finite Element Method (FEM) simulations in our recent work, indentifying scallop geometry as main cause for stress reduction [9].

In this work, we further improve on the understanding of the scallops' role in stress distribution. Our goal is not only to provide a better explanation for the stress reduction, but also to learn how the scallops geometry influences the stress and the mechanical stability of an open TSV technology.

## 2. Problem description

The presented integration technology uses wafer bonding and TSVs in order to integrate low output sensors with their associated analog amplification and signal processing circuitry (Fig. 2). Metalization and $SiO_2$ passivation are deposited conformally on the TSV surfaces following the Si etch process. More processing details can be found in the work of J. Kraft et al. [6]. At the TSV's wall, scallops – which are inherited from the Bosch process – are observed (Fig. 5b). The metal layers are composed of two double layers consisting of tungsten (W) and Ti/TiN thin films with 10 $\mu$m and 1 $\mu$m thicknesses respectively. This structure is an approximation of the one used in real devices and it is used only for simulation and study purposes.

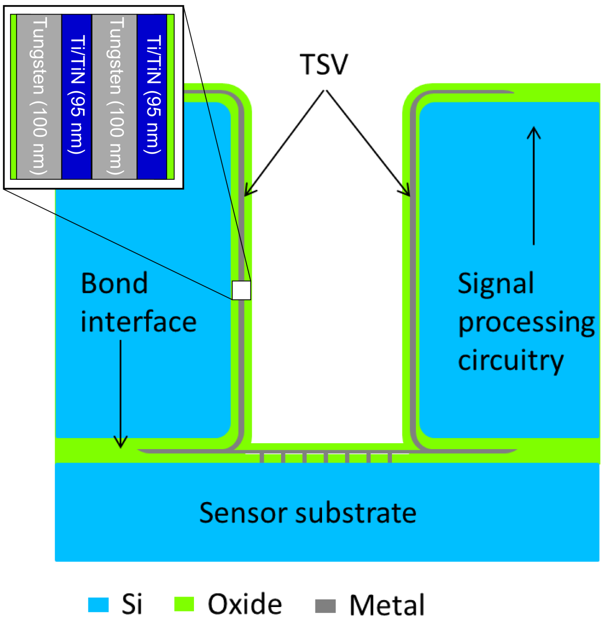


Figure 2. Schematic cross section of the open TSV technology used in this work. Metal layers composition and thickness are depicted on detail.

C. Krauss et al. performed X-Ray Diffraction (XRD) stress measurements on the metal layers of this structure [7], but the specific TSV geometry has allowed for the measurements only up to the top 10 $\mu$m. A full plate sample with an identical layer profile is then used to support stress characterization (Fig. 3). The purpose of the full plate is to ease the measurement process and to improve its precision. Additionally, full plate measurements are the best estimate for the stress in the middle of the via since it is unfeasible to probe deeper into the TSV. However, the stress on the via metal film was found to be smaller than in the full plate samples. So far, the scallops geometry still remain as the most probable cause for the stress reduction. In this paper, we followed this line of thought and, by means of FEM simulations the stress development under the influence of Bosch scallops is described.

## 3. Simulation setup

Our simulation setup is based on the structures depicted in Fig. 4. The single stacked structure (Fig. 4a) is used only for setup verification with experimental results, since there is no available data for double stack vias (Fig. 4b).

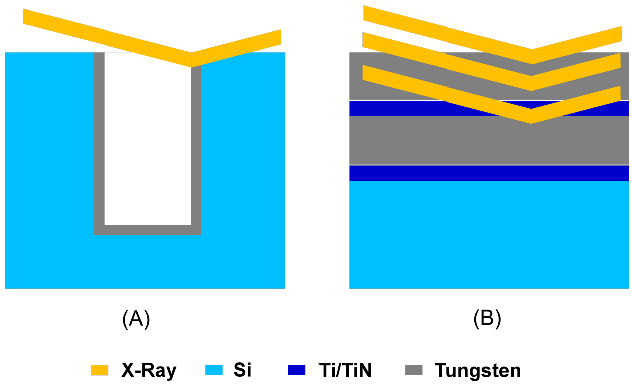


Figure 3. X-Ray measurement for TSV sample (A) and full plate sample (B). The geometry of the TSV prevents good penetration of the x-rays on the tungsten layer, therefore full plate samples are needed for better analysis.

We simulated parabolic-like scallops in several combinations of height and width. The purpose of this approach is to assess how the stress is distributed as the scallop shape is varied, so then a explantion for the reduction mechanism can be provided. The scallops height and width (Fig. 6) were varied up till 0.5 $\mu$m and 2.0 $\mu$m respectively.

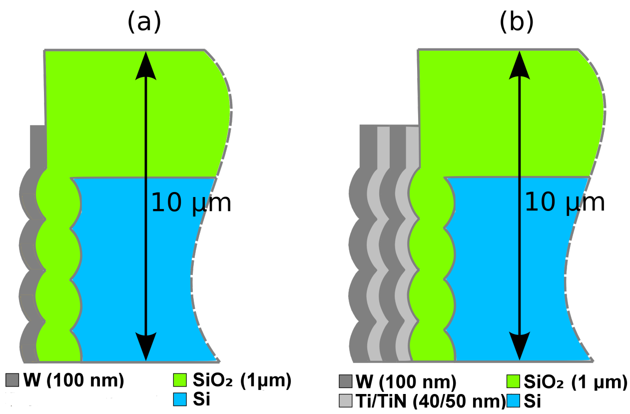


Figure 4. (a) Single stack structure used for validation simulations. (b) Double stack structure with all layers present

An accurate evaluation of our simulation results relies on a good description of the scallop's shape. Thus, the Bosch process on the TSV was simulated using an in-house Level Set based process tool [10] (Fig. 5a), but due to the computing time required it was unfeasible to go through each possible dimensional configuration. Thus, a single simulation was carried out and based on it an entire set of structures were manually constructed for several dimensional combinations.

The scallops of the considered TSV presented a parabolic-like shape as depicted on the cross section

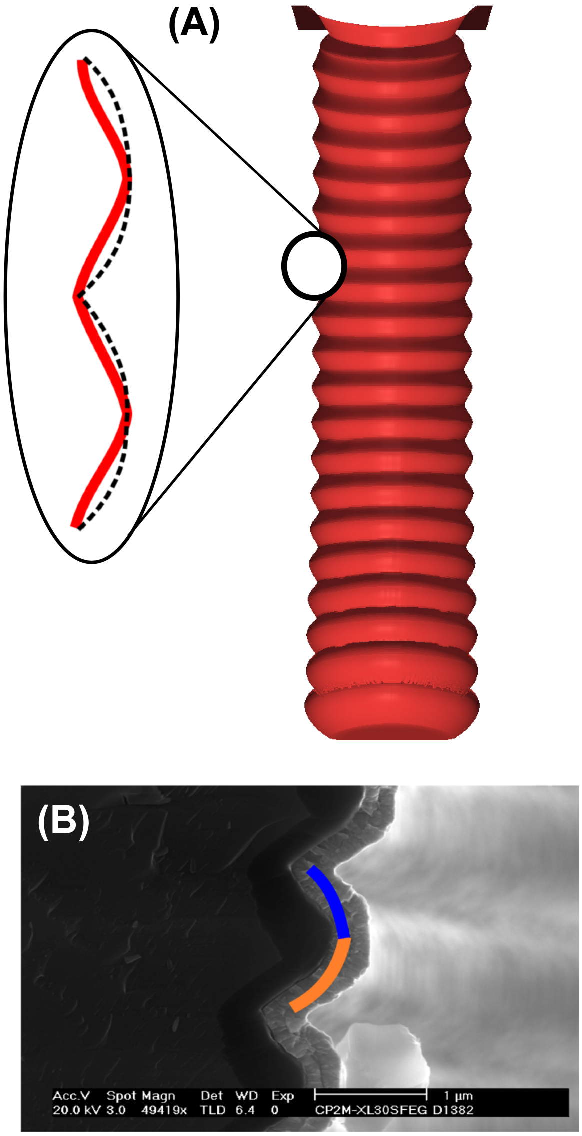


Figure 5. (A) Level-set simulation of the scallops on TSV's wall. In detail is shown how a quadratic Bézier curve compares to (dotted line) the simulated surface (solid line) (B) Scanning Electron Microscopy (SEM) image of the TSV's wall with a Bézier curve (solid line) for comparison.

TSV's images (Fig. 5b). The height and width is estimated to 2 $\mu$m and 0.25 $\mu$m respectively. The scallop's shape is approximated in our simulation by rational quadratics Bézier curves [11] which the general form is given by Eq. 1.

$$B(t) = \frac{(1-t)^2 P_0 W_0 + 2t(1-t)P_1 W_1 + t^2 P_2 W_2}{(1-t)^2 W_0 + 2t(1-t)W_1 + t^2 W_2} \quad (1)$$

Where P0, P1, and P2 are control points as depicted in Fig. 6. W0, W1, and W2 are weights used for curvature control and t is the curve parameter that varies between 0 and 1.

Two Bézier curves were used to form a scallop (Fig. 6). For each scallop, the curvature, size and width were controlled by a suited chose of weights and points relation of both curves, following the rules below

- P1 and P6 must be on the intended TSV wall (without scallops) and the distance between them defines the scallop's width.
- The distance between P1 and P2 defines the maximum scallop's height which is reached at the middle of the scallop's width.
- P1 and P2 are placed on the same side of the scallop and P5 and P6 are placed on the opposite side of the scallop.
- The weights W1, W3, W4, and W6 have the value 1. The weights W2 and W5 have the same value (which controls the scallop's curvature), W2=W5=W. We have chosen W=1/3.

Although our approach describes scallops in a parabolic form, the junction between scallops is smoother than the Bézier curve can represent. This could lead to singularities during simulation, resulting in high stress at those locations.

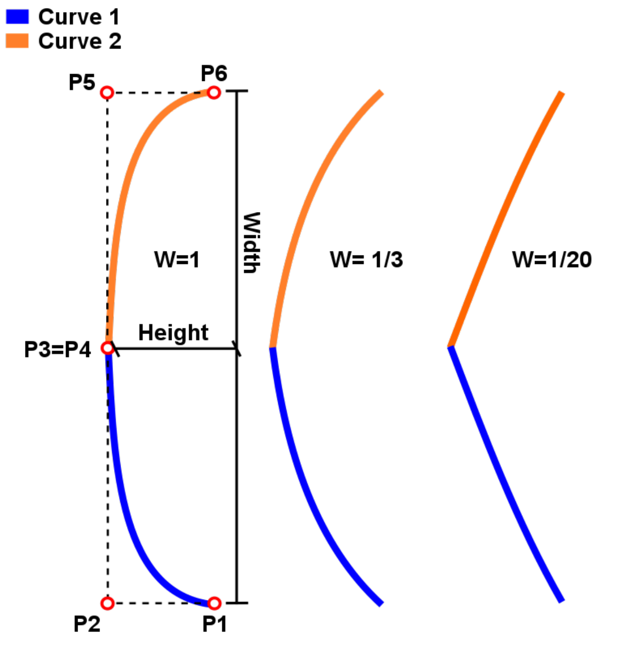


Figure 6. Representation of scallops by Bézier curves. W controls the shape of the curve and each curve is defined by three points.

The simulation of the entire structure (as depicted in Fig. 2) is computational unfeasible in the presence of a great number of scallops. Hence, we reduced the simulation domain (Fig. 7) taking into consideration the aforementioned experimental constraint (10 $\mu$m from the top of the TSV).

As boundary conditions we assumed the far right side of the structure is fixed, while the TSV's inner side and the top surface are free to move (Fig. 7). The bottom boundary has a more complicated scenario, because a proper condition is unknown in the adopted domain. To handle this situation we used symmetric boundary conditions (Fig. 7). Although this is not valid when the whole structure is considered, it is a good approximation for the geometry within the simulation domain. Additionally, it reduces any possible boundary effect which could impact the solution. The simulation was performed over an axisymmetric assumption to capture the cylindrical shape of the TSV and an initial intrinsic stress was assumed according to the experimental data on full plate samples [7].

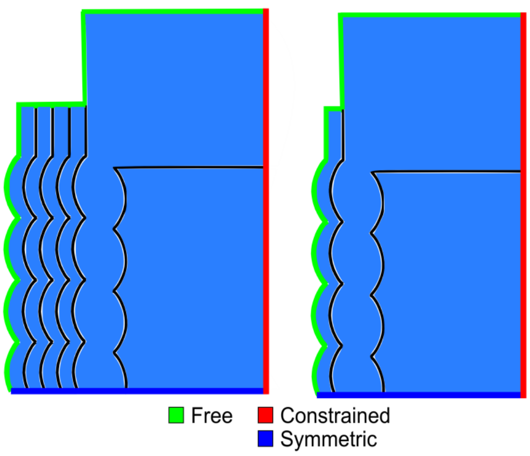


Figure 7. Simulation domain for both structures (double and single stack, respectively). The boundary conditions are also indicated.

The scallops shape demands a fine mesh to prevent numerical procedure convergence issues. As a result the mesh is rather complex near the scallops, leading to big meshes for a relatively small structure. Triangular elements were used because they showed a better adaptability in this structure in comparison to quadrilateral elements.

## 4. Results

Our first step was to validate the simulation setup, therefore the single stacked structure is considered (Fig. 8). The strain is used as target to compare the computed and experimental result, as it is a direct measure and free of any premise. The average simulated strain of 0.00169 in the z-direction was in reasonable agreement with the measured strain of 0.00111 [7] for the tungsten layer. We neglected the intrinsic stress on Ti/TiN layers due to the lack of experimental data available at the time of this publication. Simulations which considered a compressive stress in the Ti/TiN layers resulted in an average strain of 0.00127 in tungsten.

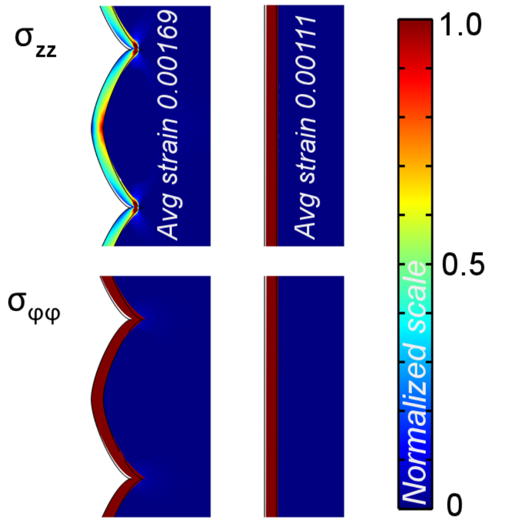


Figure 8. In-plane stress simulation of the TSV with (left) and without (right) scallops.

Hence, the absence of the intrinsic stress on Ti/TiN can justify the difference between simulated and experimental data. Additionally from the single stacked structures it is already possible to perceive the stress reduction due to the scallops. The rugosity (small-scale variation) characteristic of the scallops in the z-direction modifies the stress distribution in the TSV's films. The tensile stress induces an inward movement in the valleys between scallops. This leads to a relief of the average stress along the via – since the material finds a favorable point to expand – but an increase in the stress along the valleys and critical points appear. The same effect is noted on the double stack sample (Fig. 9).

After setup validation, critical points were identified by Von Mises stress analysis on double stack structures (Fig. 10). The mean values expose an insignificant difference (~5%) between structures with and without scallops, thus the full plate sample measurements could be used safely to estimate the average Von Mises stress. However, the mean value is not sufficient for the analysis of the structure stability when the scallops are present, due to the changing stress distribution. At the locations of accumulating stress (Fig. 10), the Von Mises stress can reach values five times higher than in full plate samples. Such high values could be the result of the sharp transition between the Bézier curves used to represent the scallops (singularity points). Regardless of the influence by the sharp transitions, these high stress points remain regions of potential failure, as increased stress could lead to a fracture in the metal.

Maximum stress magnitude varies in a peculiar way depending on the scallops height and width (Fig. 11). As the height increases, the stress increases very rapidly until a peak is reached, then it drops slowly toward a saturation

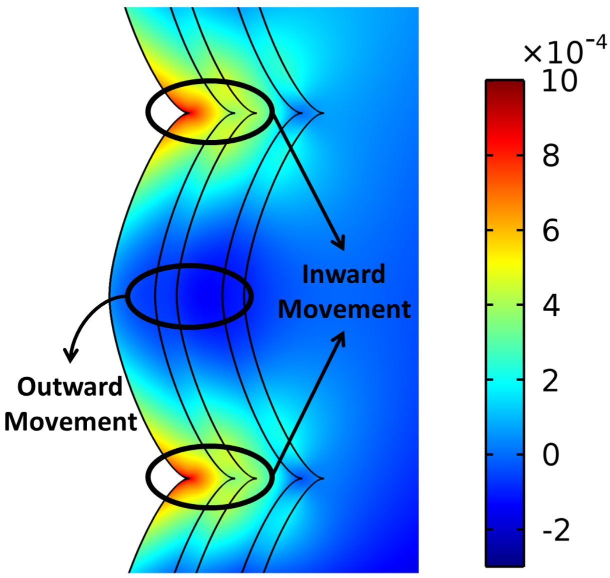


Figure 9. Displacement in R-direction.

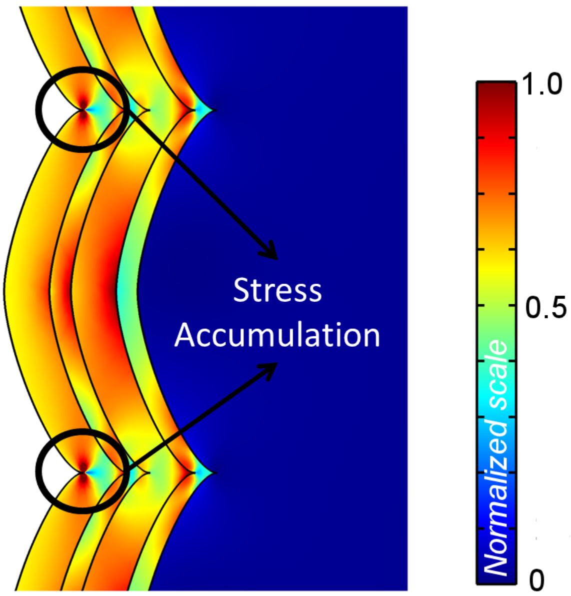


Figure 10. Von Mises stress on double stack structures. The scale is saturated for better visualization.

value. For small heights most of the scallop still retains its flat geometry (Fig. 12). This characteristic impedes material expansion and leads to stress increase. This scenario persists until the scallop reaches a height which favours the curvy geometry and the material expansion (flat characteristic is no longer dominant) resulting in stress relaxation. The peak stress in Fig. 11 is defined by this change in the scallops geometry. As the scallops' width is increased, the peak broadens with a linear dependence, both in the height and width directions. This peak movement is a consequence of the fact that wide scallops need higher heights to lose their flat behavior.

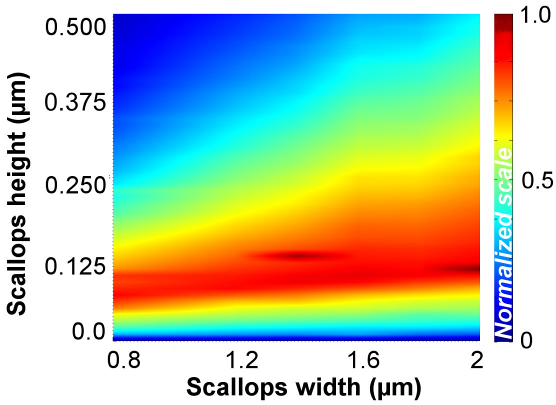


Figure 11. Maximum Von Mises stress variation according to height and width of the scallops.

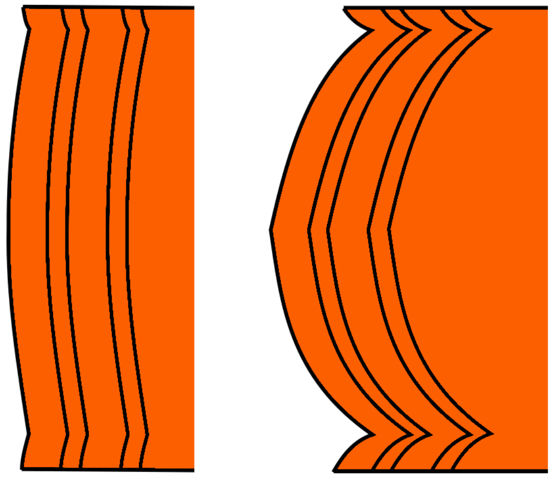

Figure 12. Flatter surface on small height scallops (left) imposes difficulties to material stretching, while curvy shape favors stress relaxation on high height scallops (right)

## 5. Conclusions

Effects of Bosch scallops dimensions on the stress in the metal layers of an open TSV technology were studied. FEM mechanical simulations were performed to identify critical points and to assess the mechanical reliability of the structure. A Level Set simulation tool was used to obtain the approximate scallops shapes and experimental results were also used to set up our mechanical simulation. We described the manner in which the scallop dimensions modify the stress. Furthermore, we explained how different heights and widths change the stress magnitude at the critical points. This information can be used to support decisions regarding device processing, especially for the etching rate and technique (isotropic and anisotropic).

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