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Stress evolution in the metal layers of TSVs with Bosch scallops

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ABSTRACT

We have studied the stress evolution in the tungsten film of a particular open TSV technology during the thermal processing cycle. The film is attached to the via's wall, where scallops were observed as a result of the Bosch processing. Our work describes a scheme which considers the scallops on the TSV and conjugates a stress model for thin-films with the traditional mechanical FEM approach. The results reveal potential reliability issues and a specific evolution of the stress in the tungsten layer.

1. Introduction

Three-dimensional (3D) integration in semiconductor technology provides an alternative for keeping the current pace of miniaturization and enhances 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 [1,2]. However, three-dimensional integration opens up new challenges in design and fabrication, which must be overcome in order to achieve large scale production [1,2].

The Through Silicon via (TSV) is one of the main elements of 3D integration technology. TSVs enable vertical connections between dies such that devices can be piled-up, thereby increasing the integration density of the technology. However, the addition of large metal vias in the middle of a die creates mechanical reliability problems. Thermo-mechanical stress arises from the difference between the coefficient of thermal expansion (CTE) of silicon and the interconnection metal. At the same time intrinsic stress arises as a result of different physical mechanisms which take place during metal deposition. Those stresses, if not managed properly, can be driving forces to delamination and cracking mechanisms, which eventually lead to device failure.

Several TSV designs were proposed as attempt to hinder the stress impact in the structure. The strategies usually involve a careful choice of the interconnection metal and via's geometry with the purpose to reduce or to compensate the CTE mismatch. Cylindrically shaped TSVs are the most successful designs, since there are no sharp corners to induce stress accumulation. An additional stress reduction can be achieved by insertion of a polymer barrier between the via and the silicon [3]. The barrier absorbs the stress and prevents its propagation towards the silicon. A different approach is the utilization of open (unfilled) vias [1,2,4]. Utilizing such TSVs 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.

The choice of the interconnection metal is a critical step of the TSV's design. The material should combine good electrical properties with low CTE mismatch to silicon. Copper is a common option due to the high conductivity of the material and the fabrication easiness. However, the difference of more than one order of magnitude between silicon and copper CTEs affects negatively the mechanical reliability. Tungsten is used as an alternative to copper, especially in TSVs for which the mechanical stress is a major concern. Although tungsten does not bear the electrical qualities of copper, the CTE mismatch to silicon is very low.

The TSV technology considered in this work uses the open via as strategy to diminish the mechanical impact in the silicon. Furthermore, the adoption of tungsten as the via metal enhances the mechanical stability of the structure for the reasons stated before. Although this TSV technology has several advantages regarding the mechanical stability of the via surroundings, the via itself presents stress related issues. Tungsten films usually possess high residual stress after the deposition process and this stress can lead to cracking of the material or detaching of the film layer and, consequently, to a TSV failure. Therefore, the understanding of the stress development in the metal layer is necessary to predict failure scenarios. We have investigated mechanical aspects of this structure in several previous papers [4–6]. Other works have explored the electrical properties [2], processing [1], and experimental mechanical characterization [7] of this technology.

Nevertheless, this open TSV technology defies the mechanical modeling of the structure. At the via's wall Bosch scallops were observed as result from the via processing and, as reported earlier, the scallops modify the stress distribution and break the equibiaxial thin film assumption [6], which is used by several thin film stress models. Furthermore, direct measurement of the stress in

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such a TSV is rather challenging and during device processing some plasticity on the thin-film metal layer (tungsten) is expected due to the thermal variations from room temperature to 500 °C.

Our goal in this work is to provide means to comprehend the deformation in the tungsten layer of this open TSV technology considering the Bosch scallops and to evaluate its impact on device mechanical stability during a thermal cycle. Therefore, we propose in this work a simulation scheme based on the Finite Element Method (FEM) to analyze the via's metal plasticity and to understand the stress behavior.

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 [1]. To assess stress in the metal layer of the structure, X-ray Diffraction (XRD) measurements were previously performed [7]. But the cylindrical shape of the TSV prevents measurements on regions deeper than 10 μm from the TSVs top (Fig. 1a). Thus a full plate sample with same layers composition and thickness is used to support characterization (Fig. 1b). The purpose of the full plate sample is to provide an estimate for the stress in the unreached deeper regions of the via. Our method is to establish based on these measurements (for the full-plate) a FEM model which can be used for evaluating the stress on TSVs' metal layers during a thermal cycle.

Krauss et al. [7] put the sample in a thermal cycle up to 500 °C at a rate of 1 °C/s and recorded the measured stress for each step. We have inferred from these data, and also from other results of thin film modeling [8,9], that the stress behavior can be explained by the dislocation glide mechanism which causes low-temperature plasticity [9]. The dynamics of low-temperature plasticity is described by the following equations:

$$\frac{d\sigma}{dT} = -M_f\Delta\alpha - \frac{M_f}{T_R}\dot{\gamma} \qquad (1.a)$$

$$\dot{\gamma} = \varepsilon_0 \exp\left[-\frac{\Delta F}{k_B T}\left(1-\frac{s\sigma}{\tau}\right)\right] \qquad (1.b)$$

σ is the stress on the thin-film, M_f is the biaxial modulus of the material, $\Delta\alpha$ is the difference between the coefficients of thermal expansion of the film and the substrate, T_R is the temperature rate, s is the Schmid factor, ΔF is the activation energy, and τ is the critical shear stress. Additionally, σ can be described in terms of the stress tensor components (σ_{ij}) by the following relation:

$$\sigma = \left(\frac{1}{2}S_{ij}S_{ij}\right)^{1/2} \qquad (2.a)$$

$$S_{ij} = \sigma_{ij} - \frac{1}{3}\delta_{ij}\sigma_{kk} \qquad (2.b)$$

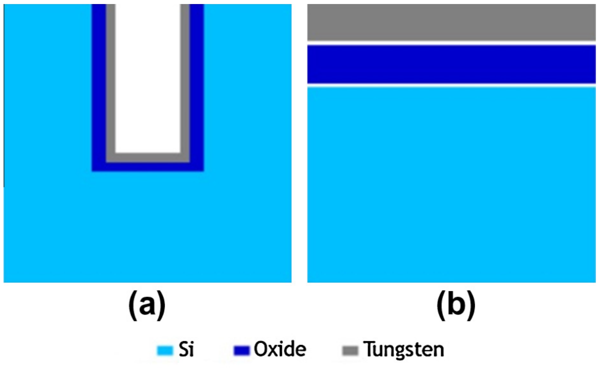

Fig. 1. (a) TSV sample. (b) Full-plate sample. Cylindrical geometry prevents the XRD measurement to reach regions deeper than 10 μm from the top. A full-plate sample with the same composition and layer thickness is used as an alternative for the measurement.

2.1. Model parameters

In order to obtain proper values of the parameters, we have fitted (1) to experimental data [7]. Since (1) is a differential equation, traditional fitting techniques based on gradient methods are not suitable. Therefore, we used a meta-heuristic optimization technique known as Genetic Algorithm (GA). Our goal was to obtain the set of parameters (M_f, ΔF, τ, s), which minimizes the distance between the experimental and the computed stress at different temperatures. Therefore, we can describe our objective mathematically by:

$$\min_{M_f,\Delta F,\tau,s} \sum_i |\sigma_E(T_i) - \sigma(T_i)| \qquad (3)$$

$\sigma_E(T_i)$ is the experimental stress measured in the temperature T_i and $\sigma(T_i)$ the computed stress by (1).

One drawback of this approach is the lack of a proof or even an evidence of the uniqueness of the solution of (3). This means that there is a chance that two different sets of parameters with different physical meaning solve (3). However, during this work we have not experienced such a situation. The obtained parameter values are summarized in Table 1.

The resulted stress evolution with the parameters of Table 1 can be seen in the next section "Section 3" in comparison with the experimental data.

2.2. Coupling with FEM

In order to have a thermo-mechanical simulation of the TSV, which properly considers the plasticity mechanism previously described in this section, (1) must be included in the thermo-elastic FEM model of the structure. The coupling has to consider the breaking of the equibiaxial thin film assumption in the TSV, consequently the stress computed in (1) has to be related to the individual stress components. The relation is given by the associated flow rule:

$$\dot{\varepsilon}_{ij} = \frac{\dot{\gamma}}{3\sigma}S_{ij} \qquad (4)$$

$\dot{\varepsilon}_{ij}$ are the strain rate tensor components. From (4) it is possible to obtain the individual components of the stress rate tensor:

$$\dot{\sigma}_{ij} = -M_f\alpha\delta_{ij} - \frac{M_f}{T_R}\dot{\varepsilon}_{ij} \qquad (5)$$

Eq. (5) is the generalization of (1.a) in order to include scenarios where the equibiaxial condition cannot be assured. In our simulation scheme the coupling is accomplished according to the following procedure:

Step 1. Perform a thermo-mechanical elastic simulation of the structure with an initial stress in the tungsten layer.

Table 1
Dislocation glide parameters.

Parameter	Value
M_f (GPa)	555.85
ΔF (J)	2.8592 × 10−19
S	0.2119
τ (GPa)	1.9655

Step 2. Calculate the stress in the tungsten for the next temperature value as described in (5), (4), and (1.b). The result of Step 1 is used as the current stress tensor to obtain σ by applying (2).
Step 3. Set the initial stress in the tungsten layer with the result of Step 2.
Step 4. If the last temperature value is not reached, return to Step 1 and repeat.

The first initial stress in the tungsten in Step 1 is taken from an experimental value measured at room temperature (residual stress after deposition). In Step 2, (5) is solved by a backward differentiation formula (BDF) method. The simulation runs through the entire temperature cycle (heating and cooling).

2.3. Scallops form

In order to model the scallop form we used Bezier curves as described in our previous work [5]. Such approach is easy to implement and it is flexible enough to model the width and height of the scallops. However, the junctions between the Bezier curves are very sharp and can introduce singularities in the simulation, leading to unrealistic stress values in those points. Further discussions about the scallops in this TSV can be found in our previous work [5]. The height and width of the scallops are estimated to 2 μm and 0.25 μm, respectively. The sketched model of the scallop approximation is repeated here for convenience (Fig. 2).

3. Simulation results

We have used two thermo-mechanical FEM simulations, one for the full-plate sample and another for the TSV itself, where the simulation domains are illustrated in Fig. 3. For both, (1) describes only the tungsten deformation while the remaining materials are considered to have simple thermo-elastic behavior.

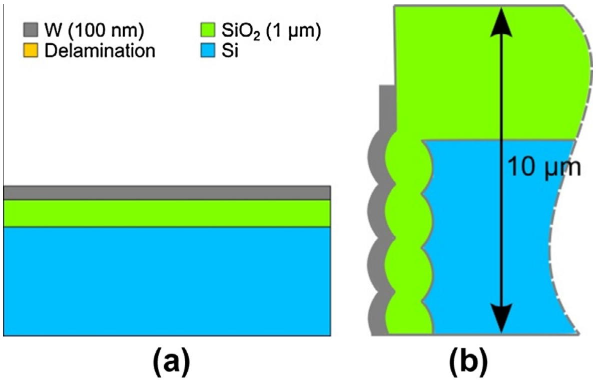

Fig. 3. Simulation domains. (a) Geometry used for full plate sample simulation. Symmetric boundaries conditions were assumed on both side borders to emulate an infinite plate and to eliminate any border effect. (b) Structure used for TSV simulation. For the analysis of the top only the first 10 μm were considered.

The purpose of the full-plate simulation is to validate the coupling between the plastic and thermo-elastic model, and also to validate the parameters in Table 1. The experience acquired through this simulation regarding assumptions, numerical issues, meshing, and physical interpretation is then applied to the actual TSV simulation.

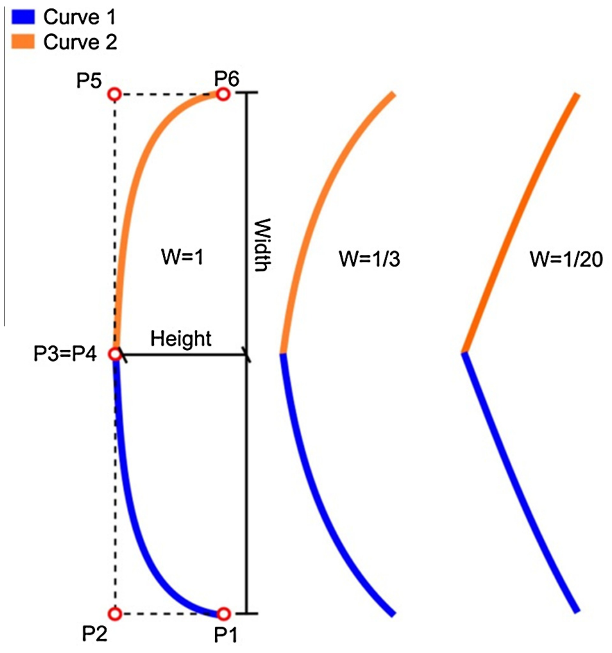

Fig. 2. Representation of scallops by Bézier curves. W controls the shape of the curve and each curve is defined by three points [5].

The full-plate simulation was set up with symmetric boundary conditions, in order to obtain a result as close as possible to a measurement carried out at the point in the center of the full-plate sample. The initial stress on the tungsten layer was taken from the experimental data [7]. The computed stress evolution follows very closely the measured values and is only slightly different from the GA fitted curve (Fig. 4). This difference can be explained by the mechanical influence of the oxide and the silicon. In such a way, the applied model, the parameter values obtained from the fitting process (Table 1), and the coupling scheme between plastic and thermo-elastic models were verified.

To simulate the stress behavior inside the TSV, an axisymmetric boundary condition was assumed. The analysis was split into two parts due to the particular geometry of the TSV. The first part concerns the top of the TSV and the second part the middle of the TSV. The simulation domain is depicted in Fig. 3b.

3.1. TSV top

The top is distinguished by the additional non-constrained surfaces regularly presented above the structure. The stress evolution at the tungsten layer is depicted in Fig. 5.

Unlike the full-plate sample, in the case of the TSV we have a highly anisotropic stress distribution. We conclude that the thermal stress in the cylindrical-shaped TSV superposes the expected stress evolution, leading to a fast decline of stress in the z-direction and a very slow growth in the θ-direction (Fig. 5). Hence, the von

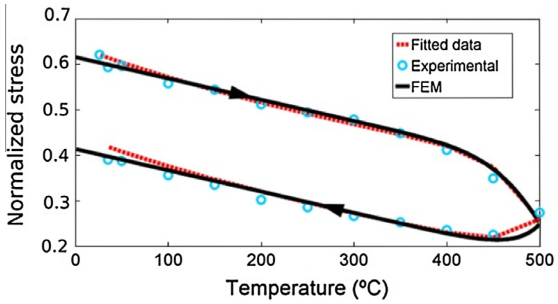

Fig. 4. Fitting result using the genetic algorithm. The differential form of (1) hinders a more traditional approach (derivative based methods), thus meta-heuristic methods are an appropriate choice considering computing costs and result quality.

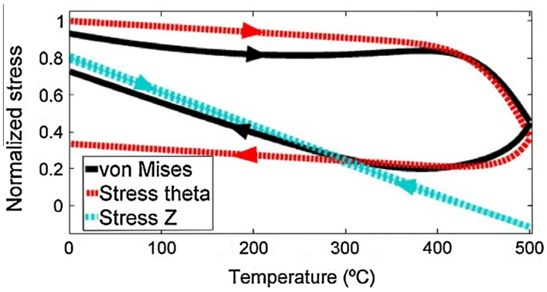

Fig. 5. Stress development at the tungsten layer in the TSV top. The original tendency for stress decline in θ-direction is contra balanced by the stress increase due to the thermal expansion, creating a plateau in the elastic region (0–400 °C). On the other hand, in z-direction the stress decline is reinforced, creating a fast decrease (almost elastic) in this direction.

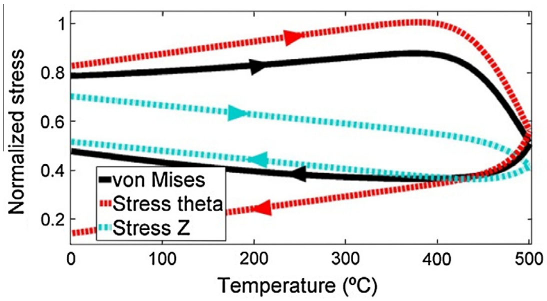

Fig. 6. Tungsten stress evolution in the middle of the TSV. During heating, the von Mises stress in the middle of the TSV increases about 10% of its initial value.

Mises stress has a peculiar behavior, during the heating it follows the upper branch of the temperature–stress curve (Fig. 5), as the stress component in the z-direction of the TSV structure does, and during the cooling it follows the bottom branch of this curve, as the stress component in the θ-direction does (Fig. 5).

3.2. TSV middle

The middle of the TSV has a different scenario in comparison to the top. The only non-constrained surface is the TSV's wall, thus the expansion of the material is more limited and consequently the overall stress increases as sketched in Fig. 6. Moreover, during heating the von Mises stress increases about 10% of its initial value, instead of decaying as in full-plate samples. Such an increase could be dangerous for the structure, since the residual stress in tungsten is already very high and an additional tension could surpass the material's ultimate strength, leading to the crack of the metal and a complete failure of the via.

3.3. Scallops role in the mechanical reliability

As reported previously the scallops induce an overall stress reduction in the tungsten and a biaxial asymmetry to the stress in the film at room temperature [5,6]. Although this scenario favors the mechanical stability of the structure, the valleys between the scallops create points of stress accumulation. These points are critical regions for the mechanical reliability of the via, at which, combined with the expected increase of the stress with temperature as discussed above, dangerous levels of tension could be reached, especially in the middle of the TSV.

4. Conclusion

We have investigated the stress development in the metal layers of open TSVs during the thermal processing cycle. We have designed a modeling methodology to include low-temperature plastic deformation by dislocation glide. Additionally, we have described a procedure to obtain the model parameters and have determined them for the tungsten layer. The simulated results are verified through comparison with experiments proving the correctness of our approach. The stress inside the TSV follows a particular evolution due to the influence of the geometry deformation during temperature variation. Finally, we have identified a critical scenario for the mechanical reliability of the structure, which is defined by the valleys between scallops in the middle of the TSV during heating of the structure.

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