Stress Evolution on Tungsten Thin-Film of an Open Through Silicon Via Technology

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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 and some plasticity is expected in the metal due to the temperature variation. Our work introduces a stress model for thin-films utilizing the traditional mechanical FEM approach. The results reveal potential reliability issues and a specific evolution of the stress in the tungsten layer.

I. Introduction

We investigated an open TSV technology based on tungsten for three-dimensional (3D) integration, which was presented for the first time in 2010 [1]. Since then, several papers have been published about its electrical [2] and mechanical properties [2-4], and, so far, the structure has proved mechanically stable and reliable.

Thermal and intrinsic stresses are responsible for several reliability issues related to TSVs. Consequently, they have become a major concern in designing mechanically stable structures [4-6]. The thermo-mechanical stress arises from the difference between the coefficient of thermal expansion (CTE) of the silicon and the interconnection metal. At the same time the intrinsic stress rises as a result of different physical mechanisms that take place during metal deposition.

The impact of stress can be controlled by the choice of the materials and the geometry which forms the TSV. A good design should manage the mechanical issues, while it ensures the electrical functionality of the device. One of the most common and well documented layouts is the cylindrical copper TSV. The good electrical properties of copper and the fabrication easiness are clear advantages of this technology. However, the difference of more than one order of magnitude between silicon and copper CTEs negatively affects the mechanical reliability.

CTE mismatch can be compensated by different strategies (Fig. 1), for instance, by usage of polymer liners around the TSV [7]. The liners work as a barrier that absorbs the stress and hinders its spread towards the silicon. Another approach is the use of an open (unfilled) TSV instead of a filled via [7-8]. 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 a particular placement of them [4]. A device has usually several vias close to each other, which can be arranged in such a way that the stress is mutually cancelled or at least reduced.

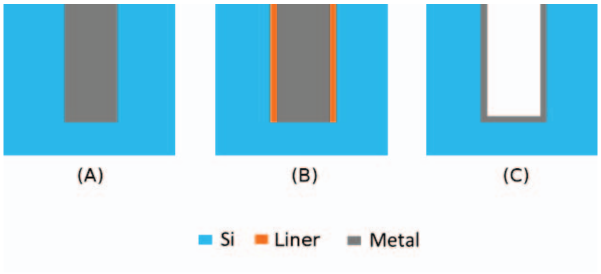

Fig. 1 – Three cylindrical TSV designs: (A) Filled TSV, (B) Filled TSV with liners, and (C) open (unfilled) TSV.

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

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stability of the structure [4], due to the low CTE mismatch between tungsten and silicon. 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.

Nevertheless, this open TSV technology defies the mechanical modeling of the structure. Direct measurement of the stress in 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 is to provide means to comprehend the deformation in the tungsten layer of this open TSV technology evaluate its impact on device mechanical stability during processing. 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.

II. 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 (c.f. Fig. 2). Metallization and SiO_2 passivation are deposited conformally on the TSV surfaces following the silicon etch process. More processing details can be found in the work of Kraft *et al*. [1].

Krauss *et al.* [3] performed X-Ray Diffraction (XRD) stress measurements on the metal layers of this structure, but to probe into the tungsten layer is difficult due to the via cylindrical geometry (c.f. Fig. 3a). Then, a full-plate sample with an identical layer profile is used to support stress characterization (c.f. Fig. 3b). 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 processing.

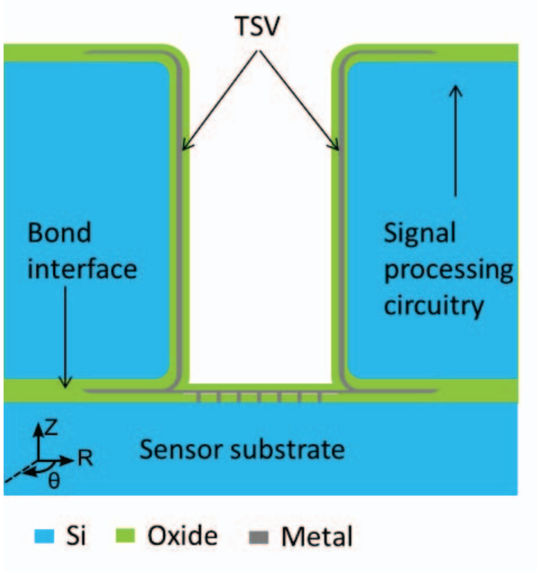

Fig. 2 - Schematic cross section of the open TSV technology used in this work.

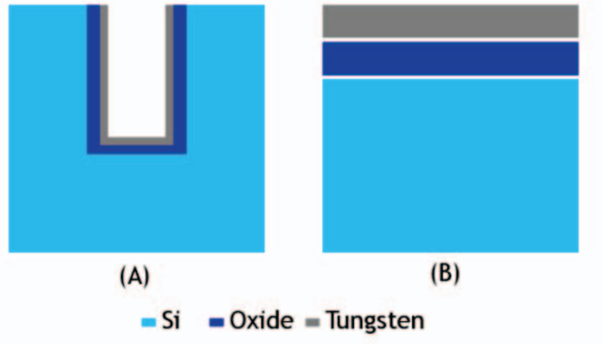

Fig. 3 – (A) TSV sample (B) Full-plate sample. Cylindrical geometry prevents the XRD measurement to reach regions deeper than 10μm from the top. A full-plate sample with the same composition and layer thickness is used as an alternative for the measurement.

Krauss *et al.* [3] 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 [10], that the stress behavior can be explained by the dislocation glide mechanism which causes low-temperature plasticity [5]. 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:

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

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

A. Model Parameters

In order to obtain proper values of the parameters, we have fitted (1) to experimental data [3]. 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, Δ_F, 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.

Table 1
Dislocation glide parameters

Parameter	Value
Mf (GPa)	555.85
ΔF (J)	2.8592 × 10-19
s	0.2119
τ (GPa)	1.9655

The resulted stress evolution with the parameters of Table 1 can be seen in the next section “Simulation results” in comparison with the experimental data.

B. 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 relate the stress computed in (1) with 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:

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

Equation (5) is the generalization of (1.a) in order to include scenarios where the equibiaxial condition for thin films cannot be assured [9-10]. 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.

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).

III. 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. 6. For both, (1) describes only the tungsten deformation while the remaining materials are considered to have simple thermo-elastic behavior.

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.

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 [3]. The computed stress evolution follows very closely the measured values and is only slightly different from the GA fitted curve (c.f. Fig. 7). 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.

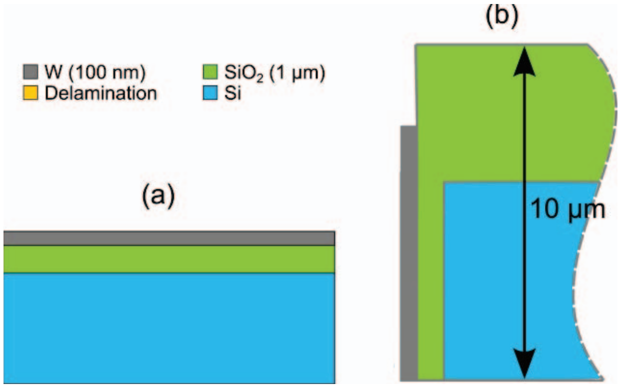

Fig. 6 – Simulation domains. (a) Geometry used for full plate sample simulation. Symmetric boundaries conditions were assumed on both side borders to emulate an infinite plate and to eliminate any border effect. (b) Structure used for TSV simulation.

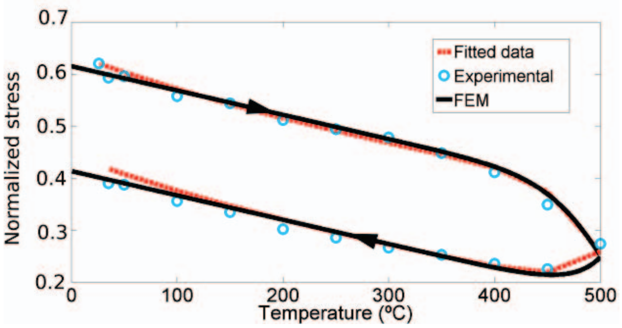

Fig. 7 – Fitting result using the Genetic Algorithm. The differential form of (1) hinders a more traditional approach (derivative based methods), thus meta-heuristic methods are an appropriate choice considering computing costs and result quality.

To simulate the stress behavior inside the TSV, an axisymmetric boundary condition was assumed. The top and the TSV's wall are considered non-constrained surfaces. The stress evolution at the tungsten layer is depicted in Fig. 8. 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 (c.f. Fig. 8).

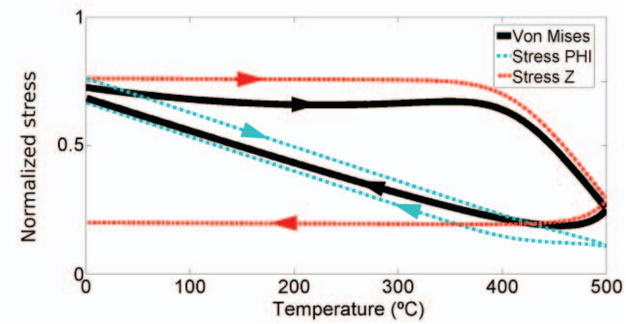

Fig. 8 – Stress development at the tungsten layer in the TSV top. The original tendency for stress decline in theta-direction is contra balanced by the stress increase due to the thermal expansion, creating a plateau in the elastic region (0-400ºC). On the other hand, in z-direction the stress decline is reinforced, creating a fast decrease (almost elastic) in this direction.

Hence, the von Mises stress has a peculiar behavior, during the heating it follows the upper branch of the temperature-stress curve (c.f. Fig. 8), 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 (c.f. Fig. 8). Moreover the Von Mises magnitude never surpasses the initial value, which can be used as estimation for the maximum stress during the thermal cycle.

IV. 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, the Von Mises stress development was exposed and the use of the initial value as maximum estimation was advised based on the simulated results. This information is vital for the proper evaluation of mechanical stability on the device.

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