2016 IEEE 66th Electronic Components and Technology Conference

Mechanical Effects of the Volmer-Weber Growth in the TSV Sidewall

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***Abstract*—Open Through Silicon Vias (TSVs) are interconnections in three dimensional technologies. The tungsten material is usually employed as conductor line and it has high value of tensile intrinsic stress. The stress generated during the deposition process needs to be studied in order to avoid the mechanical failure of the TSV. We simulated the tungsten Volmer-Weber growth for a full plate sample. Subsequently, the sidewall area of the Open TSV was investigated. Due to the etch process, a formation of a surface roughness along the sidewall, called scallops, characterizes the Open TSVs. This particular structure lead to a different stress distribution in the tungsten layer. We reproduced the tungsten growth process on a scallops surface demonstrating an important decrease of the film stress compared to the full plate sample. The simulations of the Volmer-Weber growth can be an important tool for the design optimization of TSV.**

***Keywords*-Volmer-Weber; residual stress; TSV; interconnections**

I. INTRODUCTION

Three-dimensional (3-D) technology is considered fundamental in order to maintain integrated circuit performance on the path described by Moore's law. In this context, TSV interconnections are used and by necessity, they have complex architectures, consist of diverse materials, and posses features of small size. The open TSV technology has been introduced in order to decrease the failure due to thermo-mechanical issues by the mismatched thermal expansion coefficients of the metal line and the silicon substrate in the TSV structures. In the open TSV structure, described in [1] the tungsten is employed as a metal layer. Due to deposition and thermal processes, the tungsten layer shows high value of tensile intrinsic stress. The mechanical stress in the conductor line is usually in the GPa range and this may lead to delamination, cracks or voiding, resulting in the line failure. Therefore, the study of interconnect mechanical reliability has an important role [2]. In particular, the understanding of the origin and the development of the mechanical stress in the thin film becomes a crucial necessity. The main source of the intrinsic stress lays in the deposition process [3], [4] itself. Because of thermo-dynamical reasons there are three different modes describing the film growth, namely Volmer-Weber, Frank-Van der Merwe, and Stranski-Krastanov [4]. Considering polycrystalline metal films being deposited onto polycrystalline or amorphous substrates, two different deposition processes are present during the Volmer-Weber growth. If the deposited metal has a higher melting point (Cr, Fe, Ti, W) the low-mobility Volmer-Weber growth will be the dominant deposition process. On the other side, the high-mobility Volmer-Weber growth takes place when the metal deposited has a low melting point (Ag, Cu, Au) [4].

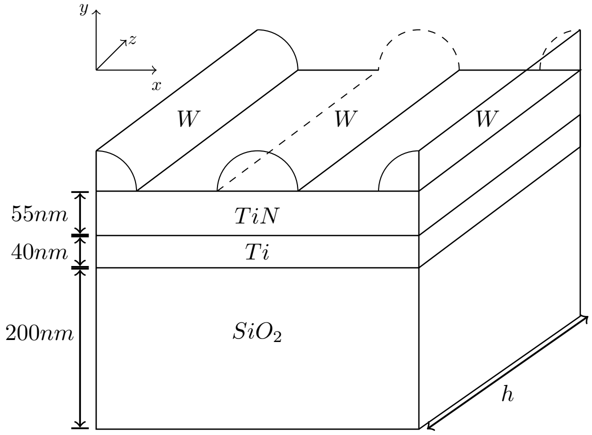

Figure 1: Schematic representation of the studied system. Full plate sample. An array of two dimensional islands with hemicylindrical shapes which coalescence was considered. Below the tungsten layer a titanium nitride and titanium layers were deposited onto a SiO_2 substrate.

In our work we considered the Volmer-Weber growth of a tungsten layer onto a titanium nitride surfaces. These configurations represent the interconnection area in the sidewall of an open TSV structure [1]. By using COMSOL Multiphysics [5], Finite Element Method (FEM) based simulations were employed to reproduce the tungsten deposition process.

During the Volmer-Weber growth three distinctive growth steps can be identified [3]. The first step is an initial growth by nucleation of discrete islands. This phenomenon can be reproduced by using the concept of the Laplace pressure. As described in literature, a compressive stress develops during this phase [4], [6], [7]. The second step is characterized by the coalescence process, where the mechanical stress is gradually changing from compressive to tensile stress. Different physical theories [6], [8], [9] regarding the de-

978-1-5090-1204-6/16 $31.00 © 2016 IEEE
DOI 10.1109/ECTC.2016.19

velopment of tensile stress during the coalescence process were proposed. Finally, the third phase of the Volmer-Weber growth is dominated by the post-coalescence process, where the formed film continues to increase until a predefined thickness is reached. Typically, for low-mobility Volmer-Weber growths, the resulting mechanical stress after all three phases of development in the film is observed to be tensile [4].

In this work, we simulated the Volmer-Weber growth by applying the three-step approach described above. Different boundary conditions as well as geometry parameters have been used in order to analyze how the stress impacts the thin film growth onto a specific substrate.

These simulations can be an important tool for the design optimization of TSV technologies and can provide a better understanding of the mechanical stress development in such structures.

II. THEORY

In microelectronics industry, material films are patterned to form electronic device. Microelectronic circuits need a fine geometry obtainable using deposition processes. The deposition process can be divided in chemical or physical where the technology used depends on the materials or the geometry of the device. The tungsten is widely employed in microelectronics and in particular in interconnections as Open TSVs. In this device the tungsten is mainly deposited through Chemical Vapor Deposition (CVD) where the low-mobility Volmer-Weber mode is the growth process [1].

The low-mobility Volmer-Weber growth was analyzed for material islands with a hemicylindrical shape [6]. The material island has been represented as half cylindrical cut along the z-axis which lays on a multilayer substrate (Fig. 1). The length of the cylinder with circular-cap cross section is infinite and this condition was reproduced using the plane-strain condition (i.e. strains in z-direction are zero) during all the two dimensional simulations.

The first step of the growth is the heterogeneous nucleation where a nucleus is formed on a surface. The minimum nucleus size formed by the atoms of the solid is indicated as the critical radius. Beyond this size the nucleus is stable and begins to grow.

In the solid nucleus, the surface atoms have an equilibrium interatomic spacing different from that of the interior atoms due to the different bonding between surface and interior atoms [7]. The surface stress f is the work per unit area required to elastically strain a solid surface A (Fig. 2). As for a free surface, a surface stress can be associated also to the solid-solid interface, between island and substrate. We indicated g as the interface stress necessary to stretch an interface by elastically deforming the island and substrate [10]. Because of the surface stress f and interface stress g a Laplace pressure ΔP will be generated. During the deposition process, the island increases in volume dV and an amount of work $\Delta P dV$. The work due to the volume increase must balance the work performed against the surface stress f and g. In this analysis we did not consider the effect of the film-substrate interface stress g [6], [7]. For positive surface stress f, a compressive stress due to Laplace pressure is observable during the first step of the deposition process [7]. By considering a hemicylindrical body, the volume V and the surface A of an island are described as

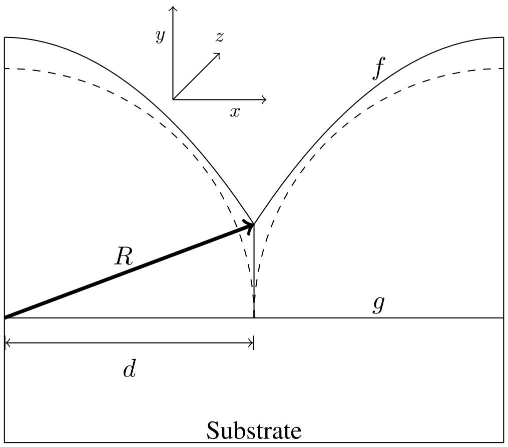

Figure 2: Schematic representation of the islands before (dashed line) and after (continue line) the coalescence.

- $V = (\pi R^2 h)/2$,
- $A_f = \pi R h + \pi R^2$,

where h is the depth of the hemicylindrical, A_f the surface related to f, and R the radius of the island (Fig. 2). For the considered geometry the Laplace pressure as a function of the volume and surface is given by:

$$\Delta P = f \frac{dA_f}{dV} = f\left(\frac{1}{R} + \frac{2}{h}\right). \qquad (1)$$

In our study the term with h is negligible for a given geometry conditions. In this first step the islands increase in radius R via deposition atoms flux due to CVD.

When an island becomes rigidly bonded to the substrate, a R_0 is defined. Above this R_0 the island is not able to release the excess of surface stress through shear stress with the substrate [7]. During the deposition, more and more adatoms attach to the island and the island grows in size. If the radius of the island is less than R_0, the nucleation does not affect the internal stress, since it is unconstrained. R_0 depends on the bond strength between island and substrate.

Therefore, since the island was rigidly bonded to the substrate when it was small, the compressive stress due to Laplace pressure in Eq. 1 develops over R_0 [6], [7]:

$$\sigma_{comp} = f\left(\frac{1}{R} - \frac{1}{R_0}\right). \qquad (2)$$

The compressive stress effects the whole deposition process, from the initial nucleation of isolated islands to the homogeneous film.

The second step of the growth is characterized by the coalescence process. During the deposition process the islands increase in volume until impingement forms the grain boundary. The coalescence leads to tensile stress generation. Considering the geometric restrictions, the average tensile stress $\langle\sigma\rangle$ generated in the film due to coalescence of material islands has been calculated applying the following equation [6]

$$\langle\sigma\rangle = \sqrt{\frac{1}{9}\left(\frac{E}{1-v^2}\right)\frac{(2\gamma_s - \gamma_{gb})}{R}}, \qquad (3)$$

where E is the Young modulus, v the Poisson ratio, γ_s the surface energy, and γ_{gb} is the grain boundary energy. This equation gives values similar but smaller than that calculated by Nix and Clemens [8] and the values obtained from it are more similar to experimentally determined by Seel et al. [6].

The third step is the post-coalescence process, where the formed film continues to grow until a predefined thickness is reached. Typically, for low-mobility Volmer-Weber growths, the mechanical stress in the film is observed to be tensile [3], [7].

III. Sample Description

In the presented work the mechanical effects of the Volmer-Weber growth for the full plate sample and for the sidewall area of the TSV structure were investigated.

The residual stress in tungsten layers either deposited as blanket films or grown along the sidewall of TSVs etched in silicon was investigated in [11]. In the full plate sample described in [11] a specific stack was deposited on the silicon substrate. The stack was composed of silicon oxide (500nm), titanium (40nm), titanium nitride (55nm) and tungsten (200nm). The Ti/TiN/W stack was repeated 2 times. For the tungsten layer on the top of the sample a grain size of 300nm ($2d$ in Fig. 2) was measured. In our model only one Ti/TiN/W stack was considered and the geometry used for the simulation calibration is shown in the Fig. 1.

At room temperature, the residual stress measured in [11] for the full plate sample was 1.6GPa. In the TSV sidewall it is 4 times smaller and was 0.4GPa. This large difference can be caused by delamination, geometry-related difference in residual stress, non equi-biaxial state of stress, and/or the presence of rippled walls in the TSV [11]. The residual stress measured is basically thermal stress, because the film is deposited at a different temperature than the operating temperature and the film and substrate have different thermal expansion coefficients. The Volmer-Weber growth occurs only during the deposition process where the stress in the film is different than the value measured at room temperature. Therefore, a FEM elastic thermo-mechanical simulation was performed to obtain the value of residual stress during the deposition process. By considering a deposition process at 400°C, obtained value was 0.64GPa. The calibration of the simulations for the full plate sample with a grain size of 300nm was estimated using the value of 0.64GPa.

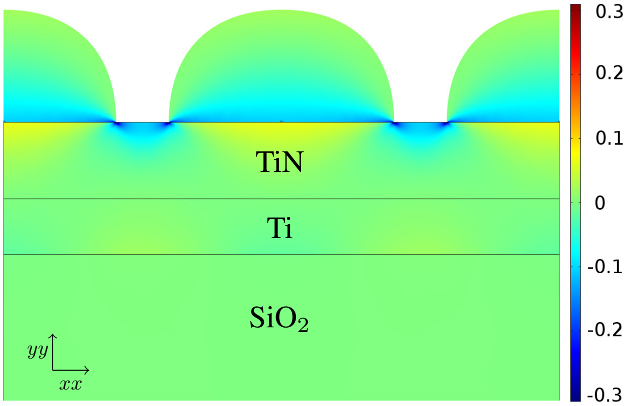

Figure 3: σ_{xx} (in GPa) during the initial nucleation of isolated islands. Development of compressive stress is observable at the tungsten islands.

IV. Full Plate Sample Simulation

A FEM analysis was employed to simulate the tungsten Volmer-Weber growth for a full plate sample. A parametric sweep study has been used to simulate the steps described in the previous sections. The variable parameter of the growth model is the island radius R which changes the island geometry during the growth. At each step a new geometry is created and a new physics is imposed. It is assumed that all materials in the simulation behave elastically and that all islands have the same size.

The first step of the growth is an initial nucleation of isolated islands. We considered the nucleus already nucleated on a surface. During the simulation, R progressively increases and a compressive stress, described by the Eq. 2, was set in the nucleus. For a full detailed analysis the simulations start with a small value of R. The parameters used are display in the Table I. The stress distribution due to the Laplace pressure during the first step of the Volmer-Weber growth is shown in Fig. 3. A low tensile stress acts on the surface of the islands and a compressive stress at the center of the islands.

The average σ_{xx} during the growth simulation was calculated from the FEM results. The measured stress is compressive (negative value) and is shown as a function of the film

f $[J/m^2]$	R_0 $[nm]$	$(2\gamma_s$- $\gamma_{gb})$ $[J/m^2]$
2.833 [10]	10	7.6

Table I: Parameters used for the simulations. The value $(2\gamma_s$ - $\gamma_{gb})$ was used as fitting parameter.

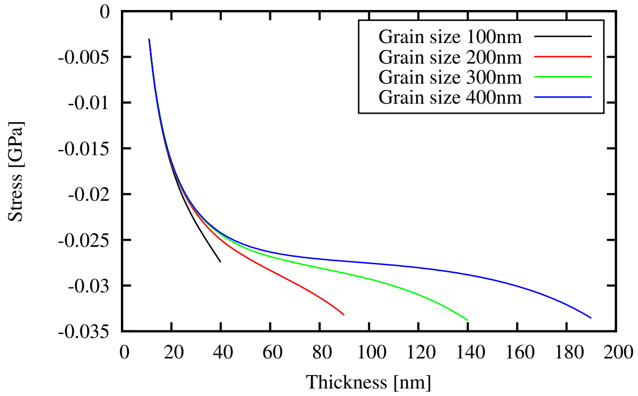

Figure 4: Behavior of the compressive stress due to the Laplace pressure for different grain sizes before coalescence. For all the samples we assumed R_0=10mm.

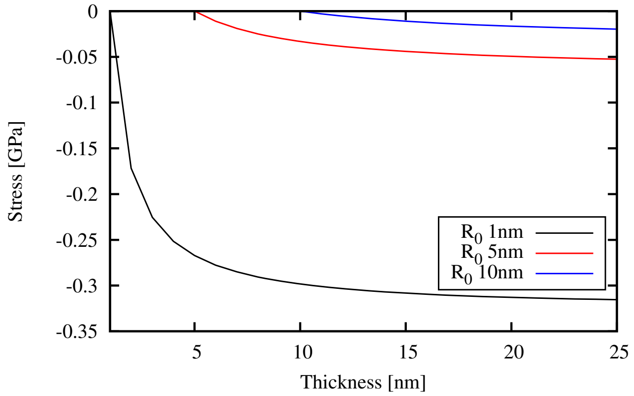

Figure 5: Behavior of the compressive stress for different values of R_0.

thickness in Fig. 4 for different grain sizes. The magnitude of the generated stress is strongly connected to the parameters used in the Eq. 2. For all the samples we assumed R_0=10nm, therefore, in Fig. 4 the compressive stress starts from the thickness of 10nm. The stress does not show big differences in magnitude for different grain sizes.

Due to the simulation condition, islands with large grain size do not impinge rapidly. Therefore an influence on the mechanical stability of the system due a longer time exposure to compressive stress in the film can be assumed. The stress originated from this process can influence the substrate (Fig. 3). If the substrate is thin and the generated stress is high the probability of crack or delamination at the interface increases [12].

From Eq. 2 we see that the magnitude of the generated stress depends on R_0. R_0 is a function of the strength of the island-substrate bonding and is assumed to be in a range 1 - 10nm [6]. In Fig. 5 different values of R_0 for the same grain size (2d=300nm) were simulated. We see that the compressive stress decreases with the increase of R_0 and the smallest R_0 produces a compressive stress around 300MPa. Stresses in this range can influence the mechanical stability of the system and in particular the thin layers. For the studied system, no values of R_0 are available in literature.

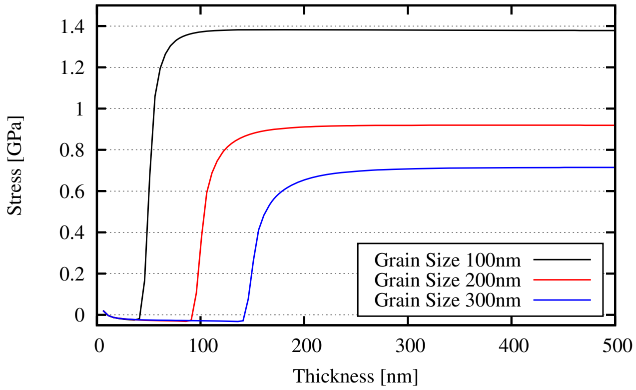

Figure 6: Average σ_{xx} dependence on film thickness for different grain size during Volmer-Weber growth. After the coalescence, the stress becomes tensile and constant.

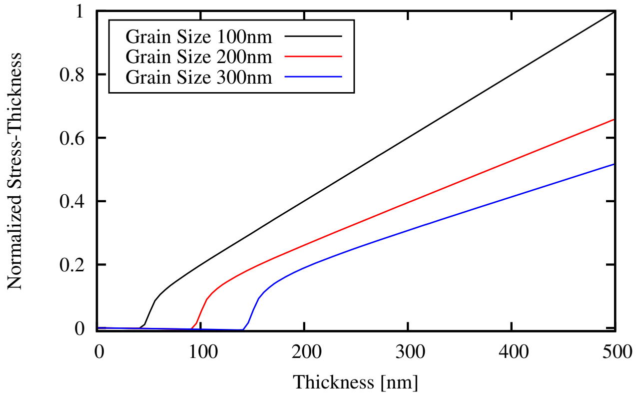

Figure 7: Normalized stress-thickness for different grain size during growth.

The second simulation step is characterized by the coalescence process, where the mechanical stress is gradually changing from compressive to tensile. The Eq. 3 was used at the first point of contact between the islands. The tensile stress is generated due to the impinge of the islands. During the coalescence process grain boundaries are formed due the atoms interactions.

We calibrated the simulation using the residual stress value of 0.64GPa (Sec. III). (2γ_s-γ_{gb}) in the Eq. 3 was varied until we obtained the average σ_{xx} desired at the thickness film of 200nm. The value used is shown in Table I. In Fig. 6 the average σ_{xx} in the film as a function of the film thickness is shown for different grain sizes. The simulations were carried out until a thickness of 500nm is

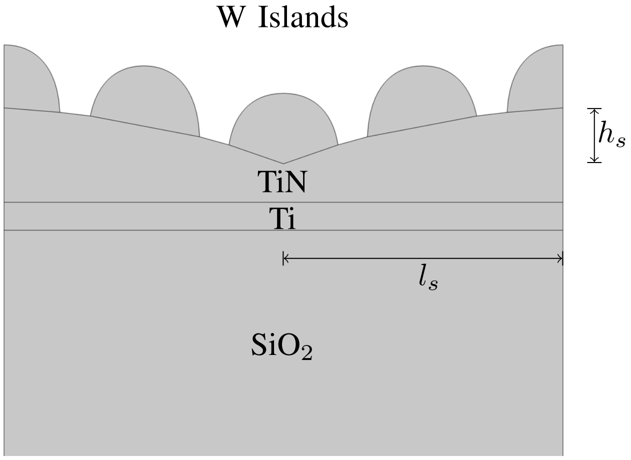

Figure 8: Geometry utilized for the growth on the scallops. On the top, two half islands and three islands were employed.

reached. At the beginning the stress is compressive, when coalescence starts the compressive stress decreases until it changes its sign and becomes tensile and subsequently it increases until reaching a constant value. The end of the coalescence process corresponds to the first peak value of the tensile stress. The Fig. 6 shows that small grain size produces high stress in the film [6].

The third simulation step is dominated by the post-coalescence process. The deposited metal has a low-mobility growth, therefore the generated intrinsic stress remains tensile during the growth [7]. In the Fig. 6 the mechanical stress in the film is observed to be constant and tensile.

The stress-thickness ($\langle\sigma_{xx}\rangle$*thickness) is mainly tensile and increase nearly linearly with film thickness. The normalized stress-thickness for different grain size are displayed in Fig. 7. This constant increase indicates the independence of the film stress on the film thickness.

V. SCALLOPS SIMULATION

The deep reactive ion etch (DRIE) [11] is an etch process used in Open TSVs technology to create deep penetration in wafers. The consequence of this technique is a scalloped TSV sidewall, which could affect the TSV performance and reliability [1], [13] as the residual stress of the film. In [11] a strong reduction of the stress was measured in the TSVs sidewall where the scallops are present. In order to understand the impact of the scallops structures on the residual stress we simulated the growth of the tungsten layer on the titanium-titanium nitride scallops (Fig. 8). The parameters employed for the simulation calibration described in Section IV were used. A grain size of 200 nm and a film growth simulation until a thickness of 400nm was performed.

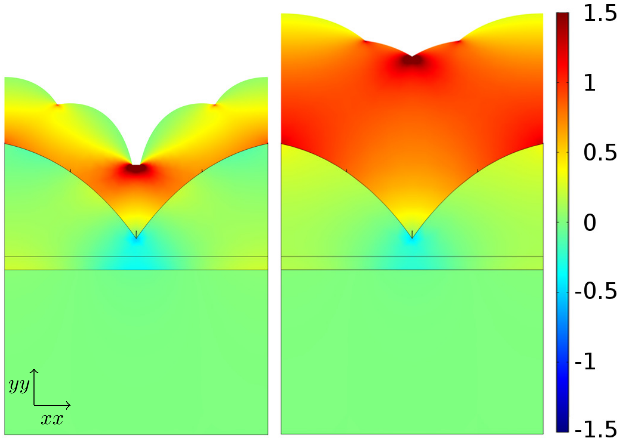

Figure 9: σ_{xx} (in GPa) in the scallops structure. The figure on the left shows the distribution σ_{xx} for a tungsten thickness of 200nm. Instead the figure on the right displays the distribution of σ_{xx} for a tungsten thickness of 400nm.

The DRIE process produces scallops with different geometry. The height of the scallops, indicated with h_s on the Fig. 8, strongly influences the stress in the film. The configuration of three islands and two half islands have been employed for simulative study. The sites of nucleation were placed on a single scallop structure with a width $2l_s$ of 1μm, as shown in Fig. 8. Three simulations with three different h_s were carried out. The Fig. 9 displays the σ_{xx} developed for a film thickness of 200nm and 400nm with h_s=0.3μm. The highest tensile stresses are observed at the intersection points of the islands. In turn, the highest compressive stress is observed at the intersection point of the scallops. These locations are the critical areas where the crack of the film or delamination can occur. Fig. 10 shows the reduction of the stress with the increase of h_s. The blue line indicates the specimen with h_s=0.3μm. Here, over the thickness value of 200nm, a rapid increase of the stress is observable. This effect is due to the island at the junction point of the scallops, which are surmounted from the neighboring islands with the increase of the thickness. For the film thickness of 200nm the values of residual stress in the film are summarized in the Table II. The decrease of the average stress in the film is mainly due to the different distribution of the stress in the scallops. The increase of h_s leads to significant decrease of the stress. This analysis proves the importance of the geometry of the device for controlling the stress in the film. Generally, from the results presented in Fig. 9 and Fig. 10 we see that the presence of scallops strongly influence the average stress in the film. For the thick scallops the average stress in the film is lower than in a full plate sample. For thicker films the spread of the stress for different heights of the scallops is not so pronounced. The difference of the stress in the film becomes crucial for small thicknesses,

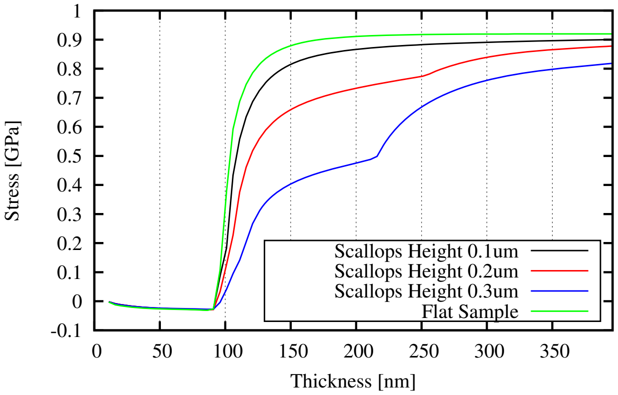

Figure 10: Average σ_{xx} for different geometries. Up to the thickness of 100nm a small compressive stress is observable. After 100nm the coalescence starts and the the compressive stress decreases until it changes its sign and become tensile.

where thin films with different heights of the scallops have significantly different value of stress.

VI. CONCLUSION

In this work we simulated the Volmer-Weber growth by applying a three-step approach. The low-mobility Volmer-Weber mechanisms of growth was implemented in COMSOL. The model facilitates study of the mechanical effects of the film growth for different geometric conditions.

In an Open TSV structure the sidewall area has as local features scallops shapes. Two different geometries, full plate sample and a TSV sidewall containing scallops, were investigated.

In Section IV we described the Volmer-Weber growth simulation for the full plate sample. The simulation was calibrated using corresponding experimental results. In the first growth step the compressive stress generated has to be considered in order to avoid a possible mechanical failure. The compressive stress depends on the value of R_0. The magnitude of the tensile stress generated at the coalescence is mainly dependent on the grain size. We simulated the compressive-tensile behavior for low-mobility Volmer-Weber growth.

In Section V, the effects of the scallops structures on the average stress of the film were investigated. Pronounced scallops lead to an important decrease of stress in the film. The average stress in the film is strongly dependent on the film thickness. In the scallops structures, the tensile stress, due to coalescence, increases slower compared to the full plate sample.

The model used for simulation enables to study the mechanical effects of the growth for different geometry conditions. The simulations performed in the scope of this work can be an important tool for the design optimisation of TSV structures and can provide a better understanding of the behaviour of mechanical stress which is relevant for the reliability of such structures.

Full Plate	h_s=0.1μm	h_s=0.2μm	h_s=0.3μm
0.91[GPa]	0.86[GPa]	0.72[GPa]	0.47[GPa]

Table II: Average σ_{xx} in the film for different h_s. An important decrease of the stress results with the increase of h_s.

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