Effects of the Initial Stress at the Bottom of Open TSVs

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***Abstract*—In this work we have studied delamination in Open Through Silicon Vias structures under different initial stress loads. The study has been carried out by means of simulation which is based on the evaluation of the J integral for different interfaces. Our simulations enabled us to determine the structures with the lowest failure probability.**

I. INTRODUCTION

Through Silicon Via (TSV) is a part of the interconnects for three-dimensional (3D) integration technology. This technology enables the development of systems with higher performance, e.g., increased density and broader functionality. TSVs are the vertical connecting devices insight the die. The usage of this new technology induces new mechanical reliability problems [1].

TSVs are cylindric structures reaching through the die. In the Open TSV technology the wall of the the cylindric hole is coated, rather than entirely filled with the conducting metal (Fig. 1)[2, 3]. Using this specific geometry can reduce the stress originating from the mismatched thermal expansion coefficients between the substrate and the TSVs materials. The bottom of the TSV consists of different material layers with different thicknesses and mechanical properties. In these interfaces the possibility of delamination leading to the failure of the device needs to be considered. The failure of the device can origin from delamination or cracking which is influenced by different parameters, such as the residual stresses or the thicknesses of the layers.

We have calculated the strain energy release rate (G) for the different interfaces at the bottom of the TSV. Considering the bottom of the TSV free to bend, cracking or delamination of the layers has to be expected under the sidewall (cf. red circled region Fig. 1). The value G is used for the prediction of the failure of the device. If the G exceeds a certain critical value G_c the interface delamination will progress. In TSVs the build up of a residual stress can occur through different mechanism: plastic deformations, temperature gradients, and structural changes.

The knowledge of the influence of initial stresses on the energy release rate can be used to limit the probability of failure of the device. We obtained the rates G for the interface for different initial stress in the adjoined layers by applyng the finite element method.

II. APPROACH

Considering a material with a crack as a straight cutting line in a body there are three different propagation modes which

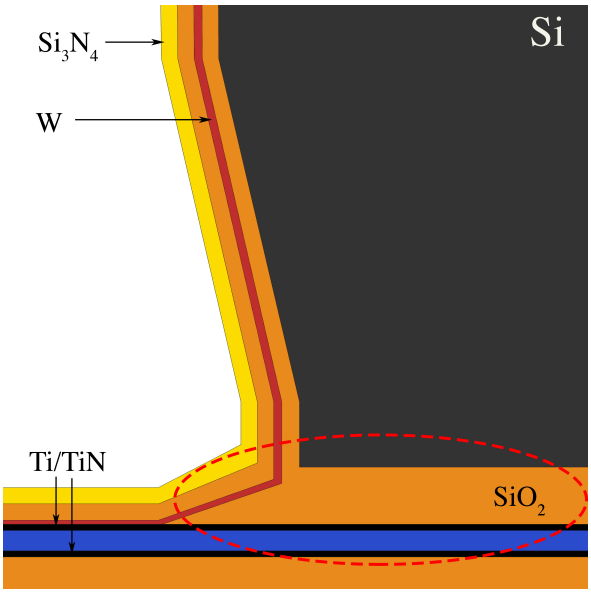

Fig. 1: Schematic of the considered Open TSV. The orange regions the SiO_2, the red the W, the yellow the Si_3N_4, the black TiN/Ti, and the blue the Al. The open TSV is integrated in the silicon of the die represented in gray. The alternating layers with different thickness are located at the bottom. There are the interfaces where a failure of the device due to delamination is expected.

are possible to define:

- Mode I: Opening, the crack opens normal to the crack plane due to a tensile loading.
- Mode II: Sliding, the crack faces are displaced on their plane, perpendicular to the crack front due to a shear loading.
- Mode III: Tearing, the crack faces are displaced on their plane, parallel to the crack front, due to an anti-plane longitudinal shear loading.

These modes can occur independently or in combination [4]. Cracks in the interface between two materials with different elastic constants are called delaminations or interface cracks. The delamination is associated with the Mode I and Mode II, moreover both modes are inseparably connected to each other [5]. For a crack or a delamination the energy release rate G is a function of the crack length and it is defined by

$$G = -\frac{\partial(U - V)}{\partial A}, \tag{1}$$

where U is the potential energy available for crack growth, V is the work connected to an external force and A is the crack

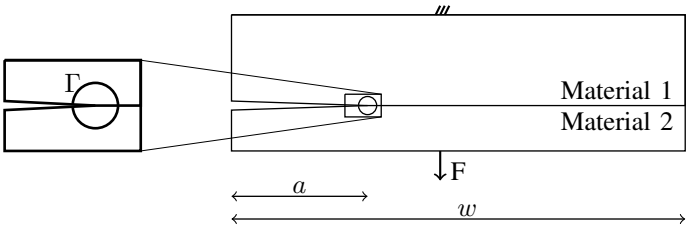

Fig. 2: Schematic representation of the studied system. In the inset the path Γ for the J integral calculation is shown. a indicates the crack length and w the width of the layer.

area. In two-dimensional problems the crack area corresponds to the crack length. The condition for a fracture to propagate is defined by

$$G \geq G_c, \tag{2}$$

where G_c is the critical energy release rate [5]. The energy release rate G corresponds to the J integral [6, 7, 8]. The value of the J integral equals the energy which is dissipated during delamination and the J integral method is applicable for system in linear-elastic fracture mechanics and also to material with inelastic behavior. It is defined as the energy per created fracture length and in delamination it is the sum of the energy released by Mode I and Mode II. The J integral is evaluated along a path Γ around the tip of the delaminated interface (inset Fig. 2). The path thereby can be arbitrary chosen as long as the interface crack tip is inside the region limited by the path [8].

The J integral is defined by

$$J = \int_\Gamma \left(W\,dy - T_i \frac{\partial u_i}{\partial x} ds \right) = \int_\Gamma \left(W n_x - T_i \frac{\partial u_i}{\partial x} \right) ds, \tag{3}$$

where W is the strain energy density, T_i are the components of the traction vector, u_i are the components of the displacement vector, and n_i are the components of the vector normal to the integration path. The strain energy density is defined by

$$W = \frac{1}{2}(\sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + 2\sigma_{xy}\epsilon_{xy}), \tag{4}$$

and the traction vector is defined by

$$T = [\sigma_{xx} n_x + \sigma_{xy} n_y, \sigma_{xy} n_x + \sigma_{yy} n_y]. \tag{5}$$

σ_{ij} denotes the components of the stress tensor and ϵ_{ij} the components of the strain tensor [7].

Considering a straight bond line the standard J integral, primarily developed for problems of single homogeneous materials, can also be applied to bi-material interfaces [8].

Two-dimensional simulations for the structure shown in Fig. 2 have been carried out. All the layers have a length of 20μm and the thicknesses of the layers has been set to the values given in Table I.

TABLE I

Layer	Ti/TiN	SiO_2	Al	W	Si
Thickness (μm)	0.05-0.2	0.4-1.4	0.5	0.1	5

TABLE II

Interface	SiO_2/TiN	Si/SiO_2	SiO_2/W
G_c (J/m^2)	1.9	1.8	0.2-0.5

All the materials are assumed to be linear elastic. We studied the failure of the interconnection in the area under the sidewall, therefore the top layer of the simulation region is assumed mechanically fixed as the sidewall of the TSV is fixed. Further a downward force is applied on the bottom of the system and the bottom of the TSV was considered free to bend (cf. Fig. 2). In all simulations the same force was applied. The simulation were started with a small initial crack length and gradually increased until a predefined value was reached.

The four interface system found in the open TSV are Ti/Al, SiO_2/TiN, SiO_2/W, and Si/SiO_2. For the prediction of failure due to delamination, the values G have been compared with critical values G_c taken from [9, 10, 11] and showed in the table II. This calculations were carried out for different ratios a/w of crack length a and layer width w. By varying the initial stresses inside the layers we have studied its influence on G.

The initial stress was introduced by setting σ_{xx} and σ_{yy} to the assumed stress values in each considered layer. The materials were assumed to be isotropic.

III. RESULTS

All simulations have been started with a crack of length 0.5μm which has been gradually increased by steps of 0.5μm untill 3μm has been reached. In all the plots shown (Fig. 3-Fig. 9), the x-axis represents the ratio a/w, the y-axis the considered initial stress, and the z-axis the calculated G.

In Fig. 3 the G values for the interface between Ti and Al are plotted. The initial stress in the Al has been assumed compressive. Inside the Ti a constant compressive initial stress of 50MPa was used. For the Ti a thickness of 0.15μm and for the Al a thickness of 0.5μm has been set. The effect of the ratio a/w on G is small compared to the influence of the initial stress. This shows that the probability of a failure is essentially reducible by a decrease of the initial stress.

Fig. 4 depicts the G value for a interface between Ti and Al where initial stress of the Ti was varied. For the Ti a thickness of 0.15μm and for the Al a thickness of 0.5μm has been set. A compressive stress of 100MPa was set in the Al layer. The reduction of initial stress in Ti leads to an increase of the energy release rate, therefore in contrast to Fig. 3 the decrease of the initial stress in the Ti layer can lead to a delamination. The increase of the crack length does not influence G significantly. For this interface no value of G_c usable to compared with our values were available in literature.

Fig. 5 shows the behavior of G at the interface between Si and SiO_2. Thicknesses of 5μm and 1.4μm for Si and SiO_2 were used, respectively. The critical values G_c was found to be 1.8J/m^2 [10]. All the points are distant from the critical value. A slight decrease of G with an increase of the crack length is

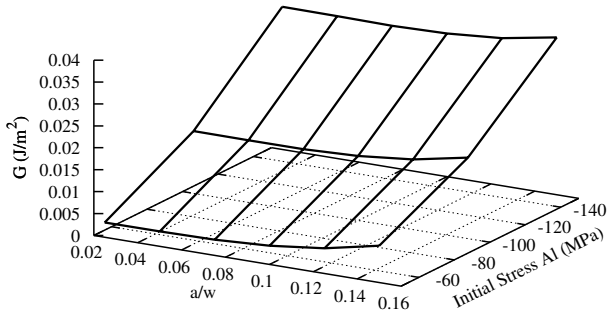

Fig. 3: The energy release rate G for different initial stresses and crack lengths in the interface Ti/Al.

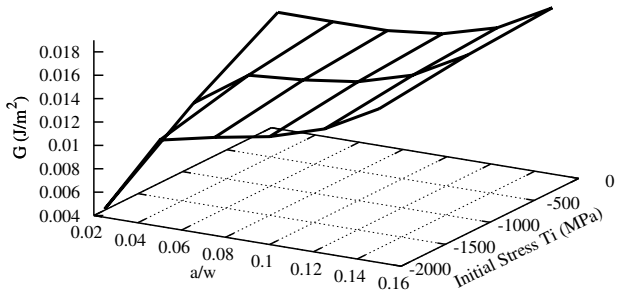

Fig. 4: The energy release rate G for different initial stresses and crack lengths in the interface Ti/Al.

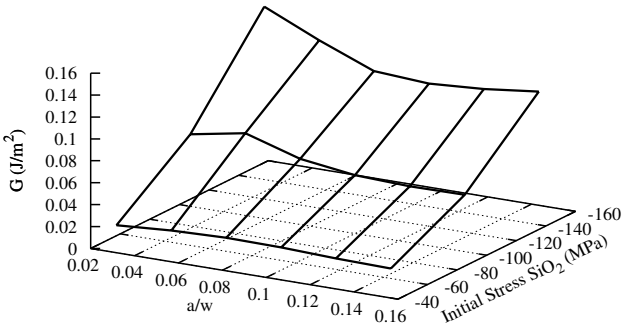

Fig. 5: The energy release rate G for different initial stresses and crack lengths in the interface Si/SiO_2.

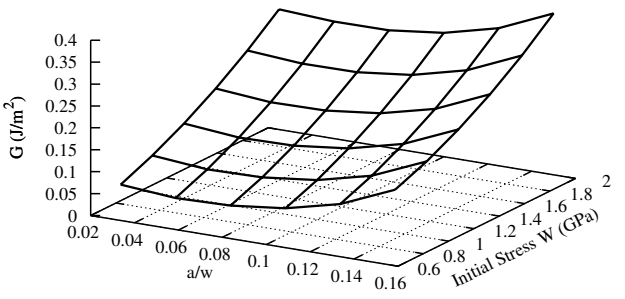

Fig. 6: The energy release rate G for different initial stresses and crack lengths in the interface SiO_2/W.

observable. This shows the stability of this interface for every crack length and for every initial stress in the SiO_2.

The behavior of G at the SiO_2/W interface is shown in Fig. 6 for a thickness of 0.4μm for the SiO_2 layer and a thickness of 0.1μm for the W layer. In the SiO_2 a compressive initial stress of 100MPa has been assumed. The simulations have been carried out for different tensile initial stresses in the W layer. The G_c according to [11] is in the range of 0.2-0.5J/m^2 and therefore small compared to G obtained for the SiO_2/W interface. For this system the influence of the ratio a/w variation is small compared to the initial stress variation. There is a constant increase of G with a raise of the compressive initial stress in the W layer. Initial stresses above 1.25GPa will lead to delamination for all ratios a/w and therefore to the failure of the device.

Also in Fig. 7 the interface SiO_2/W has been taken in consideration. An initial tensile stress of 1.25GPa and a thickness of 0.1μm were used for the W layer. We have simulated different compressive initial stresses in the SiO_2 using a thickness of 0.4μm. An increase of G is observable for increasing crack lengths a. In contrast with the behavior of G due to a different initial stress in the W layer, here the variation of G with respect to the variation of the initial stress in the SiO_2 is negligible. Only for high crack length the G is close to the G_c. Therefore the main influence to the stability of this interface is connected to the crack length.

Fig. 8 shows the behavior of G at the interface SiO_2/TiN. Here thicknesses of 1μm and 0.15μm for the SiO_2 and TiN are used, respectively. A compressive stress of 100MPa was used for the SiO_2 layer. Critical value G_c for this interface was found to be 1.9J/m^2 [9]. In this configuration the ratio a/w does not cause the failure of the interface. The main effect that can be the cause of problems in this interface is the initial stress in the TiN. A constant increase of G related to the initial stress can be observed.

In Fig. 9 the SiO_2/TiN interface has been analyzed. The thickness of 1μm for the SiO_2 layer and 0.15μm for the TiN layer with a compressive initial stress of 50Mpa for the TiN has been chosen. By varying the ratio a/w we found in the range of 0.08 to 0.1 a minimum of G for high initial stress. This behavior shows for a small and big crack lengths an high G. This means that the presence of a crack in the interface does not support the propagation provided the length of the initial crack does not exceed a certain value. For the chosen

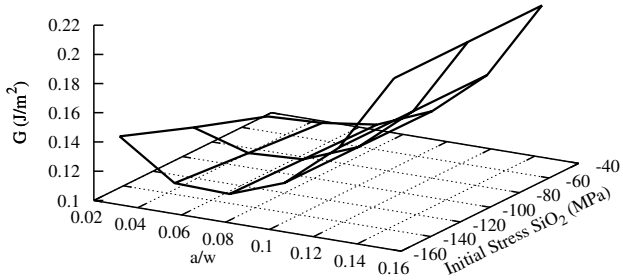

Fig. 7: The energy release rate G for different initial stresses and crack lengths in the interface SiO_2/W.

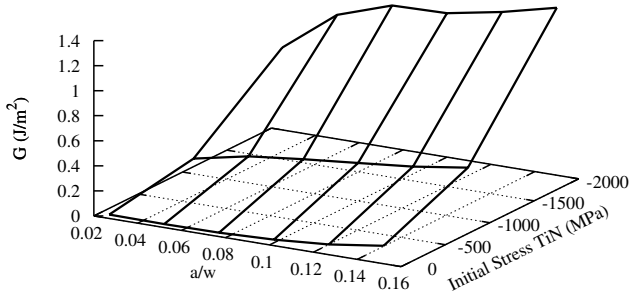

Fig. 8: The energy release rate G for different initial stresses and crack lengths in the interface SiO_2/TiN.

configuration and loads, a delamination will not occur as the values of G are below the critical value.

IV. CONCLUSIONS

In this work we have simulated the energy release rate for different interfaces. We have compared these values to the critical energy release rate G_c found in the literature to predict the probability of delamination under the chosen conditions.

In the SiO_2/W interface the delamination will occur when high values of initial stress in the W are used, or for high crack lengths. The SiO_2/TiN interface shows the possibility of delamination only for high values of compressive initial stress in the TiN layer. The variation of initial stress in the SiO_2 does not lead to values of G necessary for delamination. Comparing the critical value G_c for the Si/SiO_2 interface with our results, this interface looks stable for every crack length and initial stress chosen. Due to the unavailability of values for comparison only a qualitatively estimation of the cracking probability at the interface Ti/Al can be given. As the obtained values are quite small, we suppose that no delamination in this interface will take place. From our simulations we can suppose

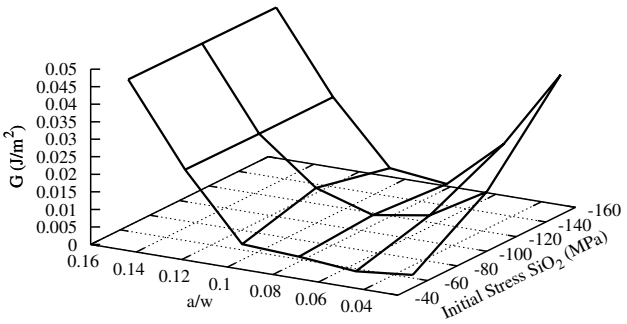

Fig. 9: The energy release rate G for different initial stresses and crack lengths in the interface SiO_2/TiN.

that the high probability of delamination will be present at the SiO_2/W interface, therefore by changing the residual stress in the W layer it is possible to decrease the probability of failure.

Results obtained in this work can help the interconnect layout designers to determine the critical fabrication processes for the open TSV, which determine the residual stress in the layers. We have shown that the effects of residual stress have a strong impact on the stability of the interfaces which are part of the TSV. The model applied in our work enables simulation of different boundary conditions (e.g. thicknesses, initial stresses, applied force) and determination of structure which would prevent delamination in TSVs.

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