Factors that Influence Delamination at the Bottom of Open TSVs

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***Abstract*—We have analyzed how the mechanical and geometrical parameters of the Open Through Silicon Vias influence failures induced by delamination of the interfaces. Through Silicon Vias are the units of the interconnection structure that establish the connection through the silicon die. We show that there are different factors that influence the failure of the device by analyzing the effect of external forces and different thicknesses of the layers on delamination. From our simulations we found how the mechanical and geometrical parameters influence the Energy Release Rate and therefore the probability of delamination.**

I. Introduction

Through Silicon Via (TSV) technology has become necessary to maintain the performance increase of integrated circuits described by Moores law [1], [2]. TSVs are cylindric structures reaching through the die. These structures are made out of different materials and are based on different design. In the Open TSV technology the wall of the cylindrical hole is coated, rather than entirely filled with the conducting metal (Fig. 1)[2], [3]. Application of this specific geometry can reduce the stress originating from the mismatched thermal expansion coefficients between the substrate and the TSVs materials. The reliability of interconnects in integrated circuits is an important issue in microelectronics. The existence of stress can be sufficient to degrade the performance, to induce crack or delamination in the TSVs [4]. The bottom of TSV consists of various interfaces between different material layers with different thicknesses and mechanical properties. At these interfaces the possibility of delamination leading to the failure of the device needs to be considered. Fig. 1 depicts the open TSV studied [2], [5], [3]. In [6] the nanoindentation was simulated to find the areas with the highest stress concentration in this structure.

The prediction of delamination for different parameters was analyzed employing the J integral to calculate the Energy Release Rate G [7], [8], [9]. Interface delamination takes place if the G exceeds a critical energy release rate G_c.

II. Approach

The study of delamination in TSVs is necessary, because the delamination can increase the probability of cracking or corrosion of conducting layer or lead to rupture of sidewall oxide isolation. To limit these problems we have analyzed how different factors can influence the delamination, and the mechanical stability of the device.

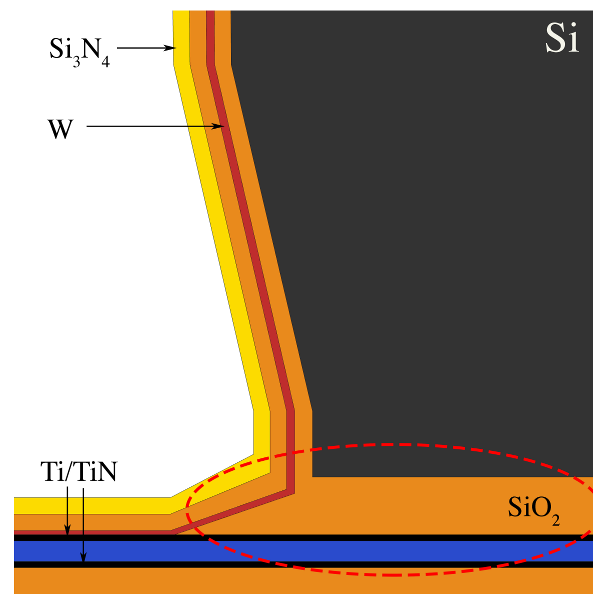

Fig. 1: Schematic of the considered Open TSV. The orange regions are the SiO_2, the red is the W, the yellow is the Si_3N_4, the black are the TiN/Ti, and the blue is the Al. The open TSV is integrated in the silicon of the die represented in gray. The alternating layers with different thickness are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

A. Failure Area

Previously we have simulated the stress development in the layers of open TSVs during nanoindentation [6]. The critical stress areas above the tip and in the corner of the TSV were identified and correspond to the places where a failure has to be expected. Cracking has to be expected in the SiO_2 and can propagate to an interface (dashed ellipse in Fig. 1) and thereon cause delamination.

B. Energy Release Rate

The prediction of delamination for different parameters was analyzed employing the J integral to calculate the Energy Release Rate G [7], [8], [9]. For a crack or a delamination the energy release rate G it is defined by

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

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TABLE I

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

where U is the potential energy available for crack growth, V is the work connected to an external force and A is the crack area. In two-dimensional problems the crack area corresponds to the crack length.

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 [9]. It is defined by

$$J = \int_\Gamma \left(W\, dy - T_i \frac{\partial u_i}{\partial x} ds \right) = \int_\Gamma \left(W n_x - T_i \frac{\partial u_i}{\partial x} \right) ds, \quad (2)$$

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

$$W = \frac{1}{2}(\sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + 2\sigma_{xy}\epsilon_{xy}), \quad (3)$$

and the traction vector is defined by

$$T = [\sigma_{xx}n_x + \sigma_{xy}n_y, \sigma_{xy}n_x + \sigma_{yy}n_y]. \quad (4)$$

σ_{ij} denotes the components of the stress tensor and ϵ_{ij} the components of the strain tensor [8]. 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 [9].

G is the energy dissipated during fracture. By comparing G with critical values G_c taken from [10], [11], [12] and shown in Table I the delamination was predicted.

The condition for a fracture to propagate [13] is defined by

$$G \geq G_c. \quad (5)$$

C. Factors

There are different factors that influence the mechanical stability of the device. These are:

- Residual stress: it was simulated adding the initial stress in each layer considered. It was introduced by setting σ_{xx} and σ_{yy} to the assumed stress values. The residual stress in the layer is due to the deposition process or the thermal process. Small changes in residual stress influence the value of G [14].
- Thicknesses of the layers: the thickness of the layer influences the G and we have used different values to find the critical condition for the delamination.
- External force: it can occur during the packaging of the device or from some human errors. We can calculate the force necessary for the failure of the device.

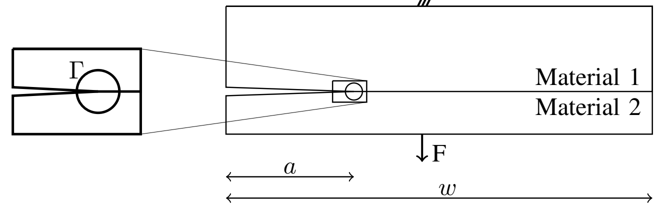

Fig. 2: Schematic representation of the studied system. In the inset the path Γ for the J integral calculation is shown. a indicates the crack length and w the width of the layer.

III. RESULTS

In the open TSV we studied four different interfaces, these are: Ti/Al, SiO_2/TiN, SiO_2/W and Si/SiO_2. G was calculated for different ratios a/w of crack length a and layer width w. Two-dimensional Finite Element Method simulations using COMSOL were employed. The structure shown in Fig. 2 have been carried out. All the materials are assumed to be linear elastic having a length of 20μm.

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 as the bottom of the TSV was considered free to bend (cf.Fig. 2). All simulations have been started with a crack of length 0.5μm which has been gradually increased by steps of 0.5μm until reaching 3μm.

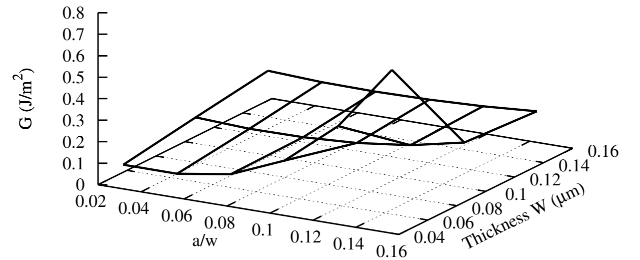

Fig. 3: The energy release rate G for different thicknesses and crack lengths in the SiO_2/W interface.

In [14] we studied the behavior of G under different values of initial stress. From our previous simulations we can assume that the delamination will most probably take place at the SiO_2/W interface, therefore by decreasing the residual stress in the W layer it is possible to decrease the probability of failure. The SiO_2/TiN interface shows probability of delamination for high values of compressive stress in the TiN layer. For Ti/Al and Si/SiO_2 interfaces we did not reach the condition for the delamination.

In Fig. 3-6 the behavior of G due to different layers

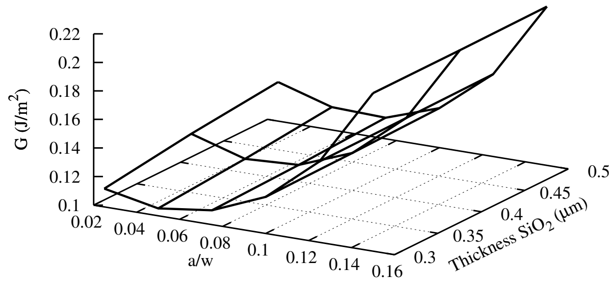

Fig. 4: The energy release rate G for different thicknesses and crack lengths in the SiO_2/W interface.

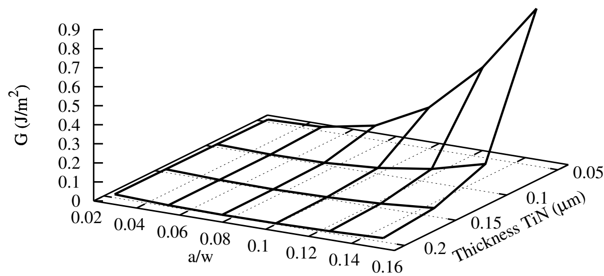

Fig. 5: The energy release rate G for different thicknesses and crack lengths in the SiO_2/TiN interface.

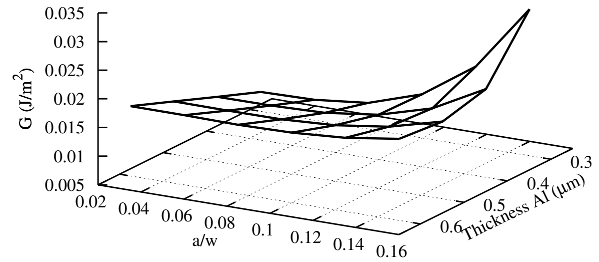

Fig. 6: The G for different thicknesses and crack lengths in the Ti/Al interface.

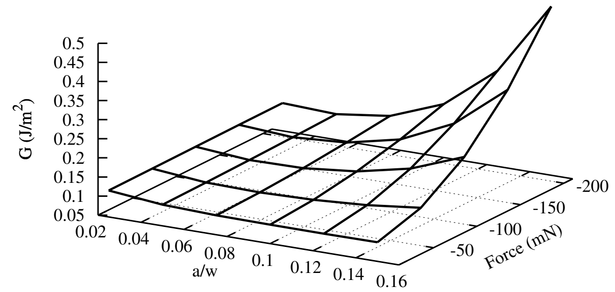

Fig. 7: The energy release rate G for different force and crack lengths in the SiO_2/W interface.

thicknesses is shown. The results for the SiO_2/W interface are presented in Fig. 3. For the SiO_2 layer a thickness of 0.4μm and a compressive stress of 100MPa was used. In the W layer a tensile stress of 1.25GPa was applied. The effect of the W thickness is highly relevant. A high increase of G is observed at long crack lengths and small thicknesses. For large thicknesses of W the calculated G is in the range of the G_c and for this condition we can expect delamination. Fig. 4 shows the behavior of G at the SiO_2/W interface. Here a thickness of 0.1μm for the W was set. A compressive stress of 100MPa in the SiO_2 layer and a tensile stress of 1.25Gpa in the W layer were used. The thickness of the SiO_2 does not have a significant influence, the increase of G is only depending of the ratio a/w. In Fig. 5 the results at the interface between SiO_2 and TiN for different TiN thicknesses are displayed. A layer thickness of 1μm and a compressive initial stress of 100MPa for the SiO_2 and a compressive initial stress of 50MPa in the TiN has been chosen. For this interface at very small thicknesses and long crack length there is an important increase of G that can exceed the G_c of $1.9J/m^2$ [12]. In Fig. 6 the interface between the Ti and Al for different thicknesses was studied. A thickness of 0.15μm and a compressive initial stress of 50MPa for the Ti was used. A compressive stress of 100MPa for the Al was chosen. The critical energy release rate for this interface is not available in literature. We can assume that the delamination will not appear because the values of G are very small. Only for small thicknesses of the Al and for high crack lengths there is an high increase of G. For the other configurations the G is almost constant.

The effects of different forces on the system are presented in the Fig. 7-9. In these simulations we have applied different forces in the range of 10-210mN. The behavior of G at the SiO_2/W interface is shown in Fig. 7. A thickness of 0.4μm for the SiO_2 layer and a thickness of 0.1μm for the W layer were employed. In the SiO_2 a compressive initial stress of 100MPa and in the W a tensile stress of 1.25GPa has been assumed. The simulations have been carried out for different forces. The G_c is in the range of 0.2-0.5J/m^2 [12] and therefore small compared to G obtained for the SiO_2/W interface. For this system only for high force values delamination has to be expected. In Fig. 8 the G values of the interface between Si and SiO_2 are plotted against the ratio a/w. An initial compressive stress of 100MPa in the SiO_2 with a thickness of 1.4μm has

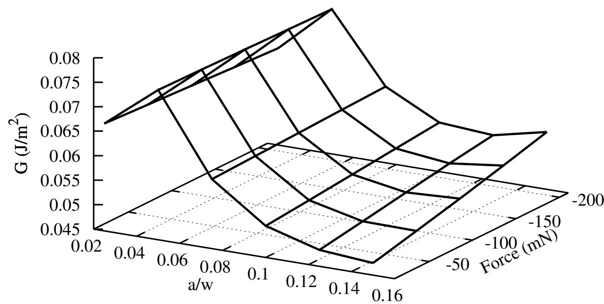

Fig. 8: The G for different forces and crack lengths in the Si/SiO_2 interface.

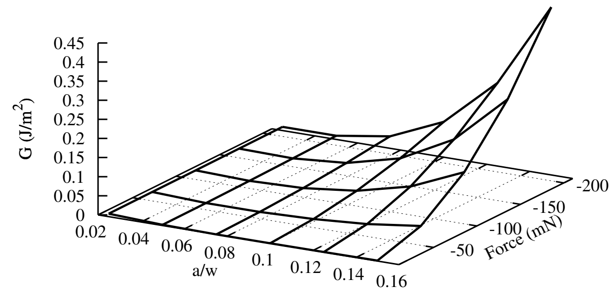

Fig. 9: The G for different forces and crack lengths in the SiO_2/TiN interface.

been used. For Si a layer thickness of 5μm has been set. The effect of a force variation is small compared to the influence of a/w. In this interface we found that for smaller crack lengths the values of G are bigger than for long crack lengths. The value G_c for this interface of $1.8 J/m^2$ [11] is much larger than that calculated. The G values of the interface between the SiO2/TiN are shown in the Fig. 9. Thicknesses of 1μm and 0.15μm for the SiO_2 and TiN were used, respectively. Compressive stress of 100MPa for the SiO_2 and 100MPa for the TiN were used. Here G raises with the increase of the crack lengths and the force applied. The values of G calculated are much lower than G_c, therefore we can expect delamination only for high force.

IV. Conclusion

From our simulations we found how the mechanical and geometrical parameters influence the G and therefore the probability of delamination.

Different values of thicknesses of the layer change the value of G. With our simulations we demonstrated that for long crack lengths the thickness of the layer has an important effect on the stability of the interface. Usually a decrease of the thickness increase G strongly. This is not applicable for the interface SiO_2/W where also at high value of thickness a high G is observable.

The increase of the force leads clearly to an increase of G (Fig. 7), but the effect is not the same for every interface. From our results it is possible to see how the force has a strong effect at the interface SiO_2/TiN (Fig. 9) than the interface Si/SiO_2 (Fig. 8) where there is a small increase of G in function of the load. We demonstrated the stability of these interfaces up to a force of 210mN.

We have shown the effects of the thicknesses of the layer and force applied. The model used in our work allows to simulate different boundary condition. These results are useful for the design optimization regarding the reduction of delamination in TSVs for 3-D integration.

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