Numerical Simulation of Thick Metal Passivation Stress, Part II: Minimizing Stress using Response Surface Methodology

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***Abstract*— In this two-part series of papers, the goal is to reduce thermal stress impact on thick metal passivation. In Part II (this paper), the relationship between passivation thickness and the thermal stress was established using Response Surface Methodology Design of Experiments (RSM DOE). Using RSM DOE, an optimum passivation thickness was determined and validated using the Finite Element Analysis (FEA) model used in Part I. The actual simulation results were close to the values predicted using statistical methods.**

Keywords*— *Finite Element Analysis; Thermo-Mechanical Stress; Back End of Line (BEOL); Response Surface Methodology

I. Introduction

It is known that cracking of passivation due to thermal stress is a major concern as cracks can cause moisture ingress, which in turn, causes metal corrosion. Aluminum metalization, which is still being widely used in BEOL layers [1], has a higher Coefficient of Thermal Expansion (CTE) than that of copper [Al: 23.1 vs Cu: 16.5 um/(m K) at 25 deg C]. This results in a higher probability for crack formation. There are also various other reasons for passivation cracking due to thick top metalization of the BEOL [2], [3], [4]. However, most efforts in this area is focused on either wire bonding [5], [6] or on wafer level solder bumping [7]. This is largely due to the fact that the silicon die is often considered as a homogenous material inside the electronic package [8]. In Part I of this series of papers, the goal was to identify the stress source that would likely cause the passivation cracking. Once the main stress cause is identified, in Part II of this series of papers, the objective turns towards determining the optimum passivation thickness that would provide the minimum stress.

II. Methodology

In Part I of this series of papers, the worst stress condition was identified to be TCT1 i.e. ramping up temperature from 25 to 175 deg C during temperature cycling. This was done using the same 3D FEA model per Fig. 1 (baseline thickness):

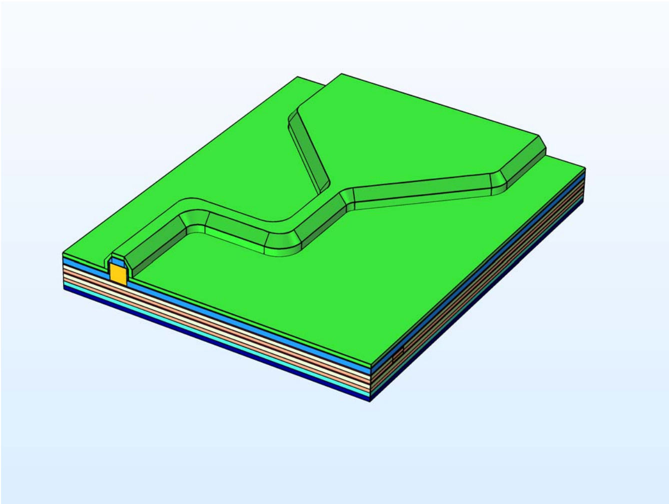

Fig. 1. Isotropic 3D FEA model showing different material layers

The Response Surface Methodology (RSM) is a multistep method attempting to fit a polynomial equation that would explain a physical phenomenon [9]. A Response Surface Methodology Design of Experiment (RSM DOE) was planned [10] to determine the optimal thickness for the three passivation layers using the worst case stress condition. For the three factors, the RSM DOE planned is a 15 run Central Composite Design (CCD) experiment [11] with eight corner points, six axial points and one centre point. Because the "experiment" is a simulation, and the results would be exactly the same for a given run, only one centre point is needed [12]. The RSM DOE plan is shown in Table I for the High Density Plasma (HDP), silicon nitride (NIT), and the Silicon Rich Oxide (SRO) thicknesses. The values are codified using Minitab as actual thicknesses are company confidential.

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TABLE I. RSM DOE THICKNESS (CODIFIED) BY PASSIVATION LAYERS.

Run	HDP	NIT	SRO
1	-1.00	-1.00	-1.00
2	+1.00	-1.00	-1.00
3	-1.00	+1.00	-1.00
4	+1.00	+1.00	-1.00
5	-1.00	-1.00	+1.00
6	+1.00	-1.00	+1.00
7	-1.00	+1.00	+1.00
8	+1.00	+1.00	+1.00
9	-1.68	0.00	0.00
10	+1.68	0.00	0.00
11	0.00	-1.68	0.00
12	0.00	+1.68	0.00
13	0.00	0.00	-1.68
14	0.00	0.00	+1.68
15	0.00	0.00	0.00

The simulation model used a linear elastic domain as the brittle passivation material would crack before any plastic yielding occurs. The model is assumed to be crack/ defect free. An optimized mesh was used where the concerned passivation layers had a higher resolution compared to other layers as these layers were susceptible to cracking. Boundary conditions included a fixed constraint at the bottom of the model.

III. RESULTS AND DISCUSSION

The output responses were the maximum first principal stress for each of the three passivation layers i.e. Max NIT_SP1, Max HDP_SP1 and Max SRO_SP1 for NIT, HDP and SRO layers respectively. The output FEA stress results from each run was collected and analyzed using a commercial statistical package, Minitab. Using Minitab's Backward Stepwise Regression function [13], factors/ terms that were not significant in changing the maximum first principal stress (Max SP1) were eliminated. Stepwise regression is an automated tool used in the exploratory stages of model building to identify a useful subset of predictors. The process systematically adds the most significant variable or removes the least significant variable during each step. The Minitab Statistical Software's backward elimination algorithm starts with all predictors in the model (in this case the thickness of HDP, SRO & NIT, two way interactions as well as the second order derivatives of each thickness) and the software removes the least significant variable for each step. The statistical software stops when all variables in the model have p-values that are less than or equal to the specified alpha-to-remove value [9], [10]. The backward stepwise method is used as this allows simplification of the regression model. The regression analysis resulted in Eq. 1, Eq. 2 & Eq. 3. It was observed that the SRO thickness is not significant in causing a change in Max NIT_SP1. However, the Max HDP_SP1 is dependant on the SRO thickness and its quadratic derivative. The Max SRO_SP1 is dependant on the NIT thickness, SRO thickness and a quadratic function of the SRO thickness.

$$\text{Max NIT\_SP1} = 0.8826 + 0.0177\ \text{HDP} - 0.3157\ \text{NIT} + 0.0964\ \text{NIT}^2 - 0.0824\ \text{HDP*NIT} \quad (1)$$

$$\text{Max HDP\_SP1} = 0.743 - 1.799\ \text{SRO} + 1.916\ \text{SRO}^2 \quad (2)$$

$$\text{Max SRO\_SP1} = 0.5772 - 0.1086\ \text{NIT} - 0.0018\ \text{SRO} + 0.1879\ \text{SRO}^2 \quad (3)$$

Previous failure analysis indicated that the crack originated in the top NIT layer. Therefore, it was important to analyze this layer in detail. Using Eq. 1, a contour plot is generated for Max NIT_SP1 (see Fig. 2).

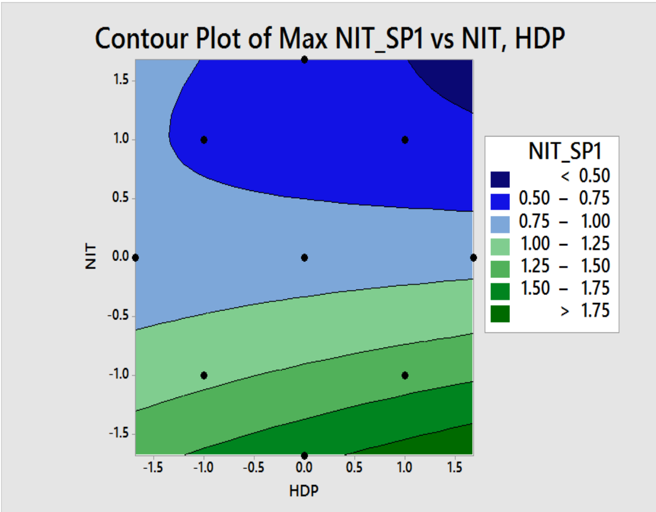

Fig. 2. Contour plot showing relationship of Max NIT_SP1 with the input factors. Black dots represent the experimental run points

As seen in the contour plot, the NIT thickness has a large influence on the Max NIT SP1 value compared to the HDP thickness. This is also reflected in Eq. 1 where the NIT coefficient's magnitude is also larger than the HDP coefficient's magnitude. The positive quadratic term for NIT thickness in Eq. 1 results in a minimum point at the top corner of Fig. 2, but this point is outside the experimental window for the Max NIT SP1 output response. The main goal of this work is to minimize the Max NIT_SP1 value for the worst stress condition i.e. TCT1. This is done by optimizing the passivation layer thicknesses. However, it is also important to ensure that the optimized thicknesses are suitable for the other passivation layers as well. Therefore, Minitab's Response Optimizer function was used to determine passivation thickness values that would result in minimum stress values for all the passivation layers. In Fig. 3, it is shown that the maximum HDP and NIT thickness would result in the minimum stress. However, an optimum SRO thickness is required for the minimal SRO & HDP stress as both these output responses are dependant on the quadratic derivative of the SRO thickness (refer to Eq. 2 & Eq. 3). The composite desirability of 1.00 indicates the settings seem to achieve favorable results for all responses as a whole [11].

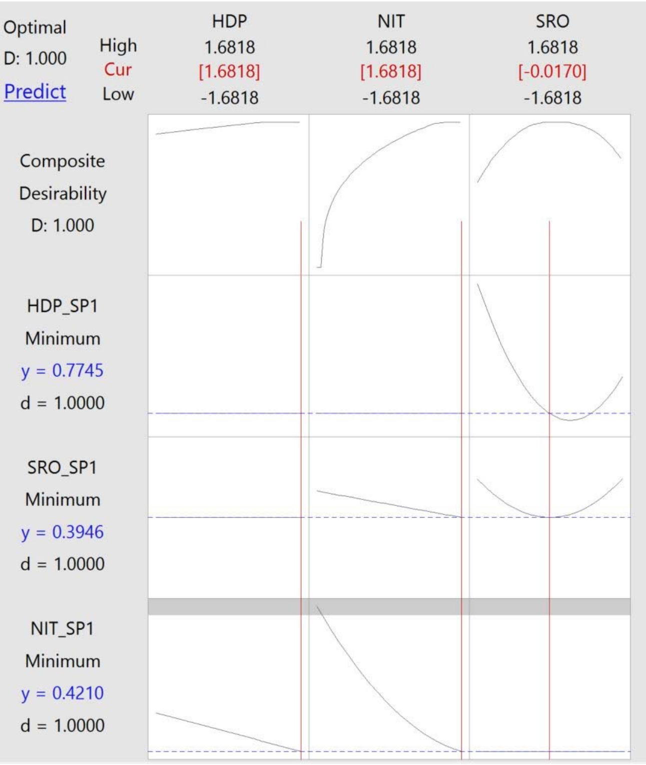

Fig. 3. Minitab's Response Optimizer showing minimum values for Max NIT_SP1, Max HDP_SP1 and Max SRO_SP1

The optimized passivation thickness values from Fig. 3 are used to predict the Maximum First Principal Stress for the passivation layers using the regression equations. The predicted values include the Fit as well as the 95% Upper and Lower Confidence Intervals (UCI & LCI). The optimized thickness values were used in the simulation model to obtain the Actual Simulation Output stress values for each passivation layer, for validation. From Table II, it is observed that both the Actual Simulation Output values for Max SRO_SP1 and Max HDP_SP1 are well within the 95% Confidence Intervals predicted by Minitab's Response Optimizer. However, the actual simulation output for Max NIT_SP1, is out of the 95% Confidence Interval bounds, but it is much lower than the stress induced on the model when it uses the baseline passivation thicknesses (see Fig. 4).

TABLE II. RESPONSE OPTIMIZER RESULTS SHOWING THE PREDICTED OUTPUT RESPONSE AS WELL AS THE ACTUAL SIMULATION VALUE WITH THE GIVEN INPUT FACTOR VALUES. VALUES ARE IN GPA.

Attribute	Max NIT SP1	Max SRO SP1	Max HDP SP1
UCI	0.707	0.679	2.912
Fit	0.421	0.395	0.774
LCI	0.134	0.110	-1.363
Actual Simulation (GPa)	0.940	0.590	0.966

When subjected to the TCT1 stress condition, the model with the baseline thickness values results in the highest stress. The RSM DOE results were used in Minitab to obtain predicted stress values for all three layers. In order to validate the Minitab prediction, the thickness values were used in the simulation model to obtain the Actual Simulation Result. All these are compared graphically in Fig. 4.

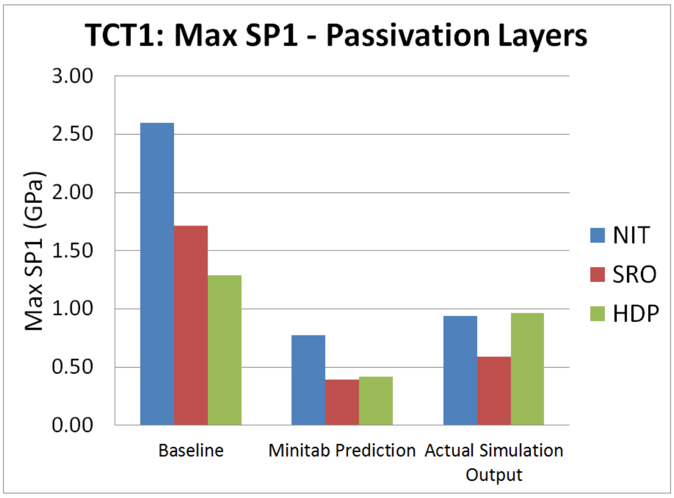

Fig. 4. Maximum First Principal Stress (Max SP1) for three passivation layers are shown

IV. CONCLUSION

In this work (Part II), it has been demonstrated that optimization techniques such as RSM DOE can minimize the stress [14]. However, such predictions need to be validated by doing a simulation with the FEA model (see Fig. 5).

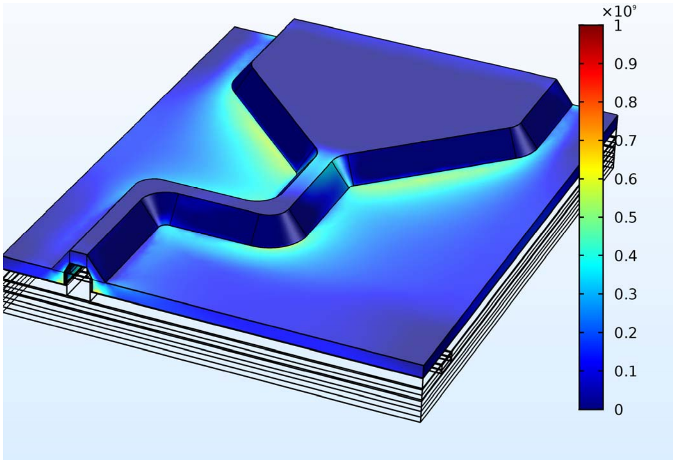

Fig. 5. Overall First Principal Stress plot for the worst stress condition TCT1 at optimal passivation thickness that results in minimum stress

Further validation using actual fabricated parts is desirable but not before doing additional simulation work as fabrication costs and time involved is prohibitive, given the limited resources. In both Part I and Part II (this paper) it is shown that a combination of FEA and statistical methods can narrow down on the possible factors that influence thermal stress and reduce possibility of passivation cracks by dielectric thickness optimization. One other method to reduce stress further is to have perforated metal designs that would allow better stress distribution into the metalization [15], [16], [17]. However this would be a subject to a future investigation.

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