Finite element analysis of influence of passivation layer on Cu/low-k structure during thermosonic Cu wire bonding

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Abstract. An incrementally coupled “mechanical–ultrasonic” finite element model, in which both the ultrasound vibration and the bonding force are considered simultaneously, is used to model the thermosonic Cu wire-bonding process on Cu/low-k structures and to study the influence of the passivation layer on the stress condition in the Cu/low-k layer. Results show that the passivation layer acts as a stress buffer layer during the wire-bonding process. The introduction of a passivation layer alleviates some of the impact effect from the free air ball (FAB). Increasing the passivation thickness can lead to significant stress alleviation. However, as the elastic modulus of passivation increases, the alleviation effect increases notably at first and then decreases.

1. Introduction
In integrated circuit (IC) manufacturing, Cu/low-k structures are being used because they have better electrical and electromigration performance than traditional Al/SiO₂ wafers [1]. However, the poor adhesion of low-k layers and the weak mechanical properties of low-k materials cause severe problems during the wire-bonding process, such as cupping, delamination, and cracks [2]. Meanwhile, Cu wire bonding is more and more widely used in wire bonding to replace traditional Au wire due to its better electrical and mechanical properties and, more importantly, its lower cost. However, because Cu is harder than Au, when it is bonded to the soft Cu/low-k structures, the problems mentioned above will be even more serious [3]. All those problems are closely related to the stress condition in Cu/low-k during the bonding process. Experiments have revealed that passivation can reduce the failure of Cu/low-k structures during wire bonding [4, 5]. However, how the passivation layer design influences the stress condition in Cu/low-k is not yet clear. In the present study, an incrementally coupled mechanical–ultrasonic finite element model is employed, taking both material softening and mechanical oscillation from ultrasound into account, in order to study the influences of passivation layer thickness and elastic modulus on stress in Cu/low-k structures.

2. Finite element model
Figure 1(a) shows the finite element mesh used in elastic–plastic finite element analysis at the initial condition. The Cu/low-k structure consists of three layers of copper metal. Figure 1(b) shows the details of the structure. In this model, the free air ball diameter is 35 μm and the wire
The displacement of ultrasonic vibration follows the following equation:

\[ Y = A_0 \sin \left( 2\pi ft \right) \]  

(1)

where \( A_0 \) is the ultrasound amplitude and \( f \) is the ultrasound frequency (120 kHz in the present study).

The Coulomb friction model is used to describe the friction involved in the wire-bonding process. The friction coefficient between the capillary and the copper ball is 0.22 and the friction coefficient between the copper ball and pad layer is 0.2 [7].

The material properties used here are listed in Table 2. The Cu FAB, Cu via, and Al plating are assumed to be isotropic elastic plastic and power laws are used here to predict the stress. The governing equation is [7]:

\[ \sigma = C\varepsilon^n \] (MPa)  

(2)

where \( \sigma \) is the effective stress, \( \varepsilon \) is the effective strain, \( C \) is the strain-hardening coefficient, and \( n \) is the strain-hardening exponent. Different values of \( C \) and \( n \) are used for Cu FAB, Cu via, and Al pad.

### Table 1. Thicknesses of different parts in finite element analysis model.

| Thickness (μm) | Al pad | Passivation | Cu Structures | Low-k | SiO₂ | Si |
|----------------|--------|-------------|---------------|-------|------|----|
| 1              | 1      | 0.5         | 2.5           | 1     | 10   |    |

### Table 2. Material properties.

| Contact body | Copper | Aluminum | Passivation | Low-k | Oxide | Silicon |
|--------------|--------|----------|-------------|-------|-------|---------|
| Elastic modulus, E (GPa) | 130 | 71 | 32 | 18 | 71.4 | 169 |
| Poisson’s ratio, ν | 0.34 | 0.33 | 0.24 | 0.3 | 0.27 | 0.3 |
| Density, \( \rho \) (g/cm³) | 8.96 | 2.7 | 2.31 | 2 | 2.2 | 2.33 |
3. Validation of FEA model

To validate the model developed, two different structures are numerically compared first. One structure includes a passivation layer directly under the Al pad and the other does not, as depicted in figure 2.

Figure 3 shows the distributions of the first principal stress and the maximum shear stress in the low-k layer [green part with the square in figure 3(a)]. The highest stresses in the pad low-k layer occur at the last ultrasound vibration cycle when the capillary’s parallel movement reaches the maximum ultrasound amplitude. For both structures, the capillary moved down 9.23 μm. The ball diameters for structure 1 and structure 2 are 38.84 μm and 39.2 μm. The bonded regions’ radii of structure 1 and structure 2 are 10.38 μm and 11.5 μm. The maximum first principal stresses in structure 1 and structure 2 are 60.77 MPa and 267.4 MPa, respectively, and the maximum shear stresses in structure 1 and structure 2 are 80.84 MPa and 104 MPa, respectively. The maximum shear stress concentration is 11 μm from the center for structure 1 and 9 μm for structure 2. For both structures, the first principal stress concentration is 11 μm from the center. It is clear than the underpad of structure 1 suffers less stress than structure 2, and thus the risk of pad damage in structure 1 is smaller than that in structure 2. This result is in agreement with the experimental findings in which the passivation directly under the Al pad strengthened the structure [4]. The predicted stresses from the finite element model developed in the present work are good indications of the tendency of underpad failure.

(a) Structure 1: with passivation layer. (b) Structure 2: without passivation layer.

Figure 2. Two different types of pad structures.

(a) Schematic of Low-k layer

(b) First principal stress of structure 1.

(c) First principal stress of structure 2.

(d) Maximum shear stress of structure 1.

(e) Maximum shear stress of structure 2.

Figure 3. Stress conditions in underpad.
4. Results and discussion

Both the experiments and the numerical predictions demonstrated the role of passivation as a stress buffer. To better design and select the passivation layer, the FE model developed was employed to study the influences of thickness and elastic modulus of the passivation layer on stress conditions in Cu/low-k structures.

4.1. Influence of passivation thickness

Stresses and distortions in a Cu/low-k structure are numerically predicted when the thickness of the passivation layer changes from 0 to 2 μm, with a constant elastic modulus of 32 GPa. The FAB is totally suppressed by a distance of 10 μm.

(a) Maximum first principal stress and the capillary descending distance.

(b) Maximum shear stress and the capillary descending distance.

(c) Radii of bonded region and the location of maximum first principal stress.

(d) Radii of bonded region and the location of maximum shear stress concentration.

(e) Pad sinking.

Figure 4. Stresses in Cu/low-k layer and pad sinking for different passivation thicknesses.
Figure 4(a) shows the maximum first principal stress and the corresponding capillary descending distance in the low-k layer for different passivation thicknesses. Figure 4(b) shows the maximum shear stress and the corresponding capillary descending distance for different passivation thicknesses. It is clear that when the passivation thickness increases, both the maximum first principal stress and the maximum shear stress decrease. The passivation thickness has little influence on the time it takes for the low-k layer to reach the maximum first principal stress and the maximum shear stress, i.e., when the capillary moves down over 9 μm and the ultrasonic amplitude reaches a maximum. Figures 4(c) and 4(b) show the stress concentration point locations and the corresponding radii of the bonded region of the maximum first principal stress and the maximum shear stress, respectively. For the first principal stress, when the passivation layer thickness is less than 1 μm, the stress concentration points are under the bonded ball; when the thickness reaches 1 μm, the concentration points are beyond the bonded region. For the maximum shear stress, all the stress concentration points are within the bonded region. Figure 4(e) presents the variation of pad sinking with increasing thicknesses of passivation. It can be seen that when a thin layer of passivation with a thickness of 0.5 μm is introduced, the pad sinking decreases significantly. When the passivation thickness is increased beyond 0.5 μm, the pad sinking first decreases and then increases slightly.

The results show that the passivation layer acts as a stress buffer layer. It alleviates some of the impact of the wire-bonding process.

4.2. Influence of elastic modulus of passivation

Stresses and distortions in Cu/low-k structure are given in figure 5 for elastic modulus of passivation ranging from 0.1 GPa to 50 GPa at a constant thickness of 1 μm. The FAB is totally suppressed by a distance of 10 μm.

Figure 5(a) and 5(b) show the variations in maximum first principal stress and the maximum shear stress in the low-k layer with their corresponding capillary descending distance for different elastic moduli of passivation. It can be seen that both the maximum first principal stress and the maximum shear stress decrease notably at first and then increase when the elastic modulus passivation increases from 0.1 GPa to 50 GPa. When the elastic modulus is 20 GPa, the first principal stress is the smallest, whereas the maximum shear stress is the smallest when the elastic modulus is 10 GPa. Also, the passivation thickness has little influence on the time it takes for the low-k layer to reach the maximum first principal stress and the maximum shear stress, i.e., when the capillary moves down over 9 μm and the ultrasonic amplitude reaches a maximum.

Figure 5(c) and 5(b) show the stress concentration point locations and the corresponding radii of the bonded region of the maximum first principal stress and the maximum shear stress, respectively. For the first principal stress, when the modulus is 0.1 GPa, the concentration point is far away from the bonded region; when the modulus is greater than 0.1 GPa, the concentration points are very close to the bonded region. For the maximum shear stress, there are no obvious trends in the locations of the concentration points. Figure 5(e) shows how the pad sinking changes for different passivation moduli.

It is predicted that the pad sinking decreases dramatically at first and then continues to decrease slightly for increased elastic moduli.

Increasing the elastic modulus of the passivation layer can lead to stress alleviation at first. However, by increasing the elastic modulus too much, beyond 20 GPa in the present work, the stress improvement will decrease.
For a passivation layer with an elastic modulus of 32 GPa, the maximum first principal stress and the maximum shear stress decrease when the passivation thickness increases from 0 to 2 μm.

The pad sinking decreases significantly when the passivation thickness increases from 0 to 0.5 μm; when the thickness is further increased beyond 0.5 μm, the pad sinking first decreases and then increases slightly.
(c) For a passivation layer with thickness of 1 μm, the first principal stress decreases notably and then increases when the elastic moduli of passivation increase from 0.1 GPa to 50 GPa. The proper value would be between 10 GPa and 20 GPa in the present study.

(d) The pad sinking decreases dramatically at first and then continues to decrease slightly for increased elastic moduli of passivation.

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