Analytical Solution for Moisture-Induced Interface Delamination in Electronic Packaging

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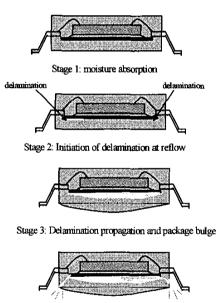
Abstract

In this paper a vapor pressure model based a micromechanics approach is introduced first, with which the moisture absorption and porosity of material, and temperature can be connected. Then the neo-Hookean model is used to describe the finite-deformation of rubber-like plastic material at higher temperature. It has been observed that the vapor pressure has almost negligible impact on the material behaviors in bulk. However, with the implementation of interface properties into the model study, it shows that the critical stress that results in the unstable void growth and delamination at interface is significantly reduced and comparable to the magnitude of vapor pressure. A framework of the description of void-growth at interface is postulated.

1 Introduction

The past decade has been marked by a substantial evolution in the understanding and modeling of the mechanics of materials at small length scales. Due to the ongoing miniaturization that has been driving the technological evolution in microelectronics and MEMS in the past years, the intriguing mechanics problems play an important role at smaller scales. For instances, the moisture-induced failure during solder reflow, often referred to the 'popcorn' failure [1], has long been considered as the consequences of the void initiation, growth and coalescence [2]. Therefore, it is necessary to introduce the micro-mechanics-based approach to investigate the problem, in order to have more profound insight into the mechanisms of the delamination failure at interface.

Polymer materials have wide applications in microelectronic packaging. Some polymer materials are used in bulk form such as encapsulant (molding compound), carrier or printed circuit boards (FR4 and BT). Some polymer materials are used as adhesives such as die-attach, underfill, or other structural and thermal adhesives. Polymers are also used in thin- or thick- film as isolation layer such as solder mask on printed circuit board or passivation layer in wafer level. Most of polymer materials, in spite of the diversities of the chemistry and compositions, are susceptible to the moisture absorption. The moisture-induced failure undergoes four different stages, which are schematically depicted in Fig. 1 [3]. In stage 1 (preconditioning), the package absorbs moisture from the environment, which condenses in micropores in polymer materials such as substrate, die-attach, molding compound and various adhesives along the interfaces. Preconditioning is a time-consuming process, and usually takes a few days or even months in controlled or uncontrolled humid environment. In stage 2, the package is mounted on to the printed circuit board by soldering. The entire package is exposed to temperatures as high as 220°C. As a result, the condensed moisture vaporizes under the sudden temperature rise associated with the soldering process. The vapor pressure and the reduction of the interface strength at high temperature due to the previous moisture intake will cause local interfacial delamination. In stage 3, the vapor pressure exerts compressive loading on the delaminated surfaces, eventually causing the package to bulge. In the final stage, a package crack forms and propagates laterally outwards. When the crack reaches the package exterior, the high-vapor pressure is suddenly released, producing an audible sound like popcorning.



Stage 4: Package cracking and vapor release Figure 1. Schamatic description of four stages of moisture-induced failures in a plastic electronic package.

The moisture exists everywhere in polymer materials in an electronic package after preconditioning. However, the rupture of *bulk* material prior to *interface* delamination has rarely been observed. The failure often starts from the interfaces through delamination, as shown in Fig. 1. The vapor pressure then exerts compressive loading on the delamination area, eventually causing the package to bulge and initiating crack branching into the bulk material.

The objective of this study is to develop analytical solutions for moisture-induced delamination failures at the interface, during solder reflow process. Previous studies [3,4, 5], in which the nonlinear constitutive relation is adopted, showed that the vapor pressure plays an important role in the delamination initiation. But the model was not able to make differences on the material behaviors in bulk material and at the interface. For instances, when elastic-plastic stress-strain relation is applied, the critical stress that leads the void collapse is 4-6 times of saturated vapor pressure, both in bulk and at interface [3,4].

This paper starts with a review of the vapor pressure evolution during the elevation of temperature. Then the neo-Hookean model is introduced to describe the rubble-like large-deformation of thermoset material when the temperature is above the glass transition temperature. The void-growth becomes unstable when the large-deformation is considered. Mechansim of a single void evolution on the interface is then postulated and analyzed.

2 Vapor Pressure Model

Previous studies assume that the moisture is always in a single vapor phase throughout the temperature rise [6], and hence the ideal gas law can be applied for the evolution of the internal vapor pressure inside voids. Since such a vapor pressure model is not linked to the moisture property of the material, it is difficult to estimate the initial or reference vapor pressure at reference temperature (e.g. temperature T_0 at preconditioning). The problem becomes very complicated when the moisture in voids is at mixed liquid/vapor phase, which occurs in most of cases for polymer materials.

One of critical issues in developing a vapor pressure model is to find out the moisture density in *voids*, denoted as ρ ,

$$\rho = \frac{\mathrm{d}m}{\mathrm{d}V_f} \tag{1}$$

where dm is the mass of moisture per unit volume of free spaces in material, dV_{f} . The moisture concentration C is defined as

$$C = \frac{\mathrm{d}m}{\mathrm{d}V} \tag{2}$$

where dV is the element volume of the porous material, which contains free spaces dV_f . It should be noted that, because of the inhomogeneous character of a porous material, the element should be established over a (finite) representative volume, RVE [2].

Introducing the void volume fraction f according to

$$f = \frac{dV_f}{dV} \quad 0 < f \le 1 \tag{3}$$

The following relation between ρ and C can be obtained

$$\rho = \frac{\mathrm{d}m}{\mathrm{d}V_f} = \frac{\mathrm{d}m}{\mathrm{d}V}\frac{\mathrm{d}V}{\mathrm{d}V_f} = C/f \tag{4}$$

Let's make a comparison of magnitude of ρ with the ambient moisture density at 85°C/85RH condition, i.e., $\rho_{ext}=0.85 \cdot \rho_g=3.04 \cdot 10^{-4}$ g/cm³. ρ_g is the saturated moisture

density. Assuming that the void volume fraction f is 0.05, and the saturated moisture concentration C is $1.25 \cdot 10^{-2}$ g/cm³ for a typical epoxy-based polymer according to the measurement by Galloway et. al. [7], equation (4) gives $\rho = 820\rho_{ext}$. This number clearly shows that how much moisture a typical polymer material could absorb. Such an amount of moisture must condense into the mixed liquid/vapor phase in material.

The following condition is used to determine the moisture state in voids at preconditioning of temperature T_0 ,

$$\begin{cases} \rho \le \rho_g(T_0) & \text{for vapor phase at } T_0 \\ \rho > \rho_g(T_0) & \text{for mixed liquid/vapor phase at } T_0 \end{cases}$$
(5)

where $\rho_{\rm g}$ is the saturated vapor density, which can be obtained from the steam table as function of temperature.

When the moisture is at mixed liquid/vapor phase, it is necessary to know at which temperature the moisture can be fully vaporized. This temperature is called the *phase* transition temperature, denoted by T_1 , which can be determined by

$$\rho\left(T_{1}\right) = \rho_{g}\left(T_{1}\right) \tag{6}$$

Now the vapor pressure in voids can be determined by the moisture state analyzed above. When the moisture is in the mixed liquid/vapor phase, the vapor pressure maintains the saturated vapor pressure p_g as function of temperature (from steam table), i.e.,

 $p(T) = p_g(T)$ for mixed liquid/vapor phase (7)

When the moisture is in single vapor phase, the ideal gas law can be followed to calculate the vapor pressure as following,

$$p dV_f = dm RT$$
 or $p = \rho RT$ (8)

Dividing both sides by dV, we obtain

$$pf = CRT \tag{9}$$

where R is the universal gas constant (=8.314J/mol).

The two vapor-phase states (p, f, T, C) and (p_r, f_r, T_r, C_r) are then related by

$$\frac{p}{p_r} = \frac{Tf_r C}{T_r f C_r}$$
 for single vapor phase from T_r to T (10)

Assuming that the material is incompressible, the change of volume element due to the temperature change is related by [3]

$$\frac{dV}{dV_0} \approx 1 + 3\alpha\Delta T \tag{11}$$

where $\Delta T = T - T_0$ and α the coefficient of thermal expansion, respectively. Thus

$$C = \frac{\mathrm{d}m}{\mathrm{d}V} = \frac{\mathrm{d}m}{\mathrm{d}V_0} \frac{\mathrm{d}V_0}{\mathrm{d}V} = C_0 \left(1 - 3\alpha\Delta T\right) \tag{12}$$

from which, it is noted that although the moisture mass is assumed conserved during the temperature rise (the desorption effect is neglected), the moisture concentration may change due to the change of the bulk volume by thermal expansion.

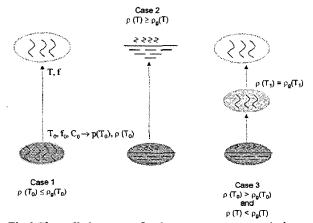
Three distinct cases for the vapor pressure evolution have been identified [2,3], and are shown in Fig. 2. In the following, the detailed description and derivation for the vapor pressure evolution for each case are presented, and some corrections on the errors in previous publications are made.

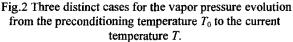
In case 1, the moisture in void is in single vapor phase at T_0 after the moisture absoprtion. The condition for this case can be mathematically expressed as

$$\rho(T_0) \le \rho_g(T_0) \tag{13}$$

or equivalently, according to equation (4)

$$C_0 / f_0 \le \rho_g(T_0)$$
 (14)





The initial vapor pressure at T_0 can be determined from equation (8), by relating with a fully saturated state at temperature T_0 , as following

$$p_{0} = p(T_{0}) = \rho(T_{0})RT_{0}$$

$$p_{g}(T_{0}) = \rho_{g}(T_{0})RT_{0}$$
(15)

thus

$$p_0 = \frac{\rho(T_0)}{\rho_g(T_0)} p_g(T_0) = \frac{C_0 p_g(T_0)}{f_0 \rho_g(T_0)}$$
(16)

by which the vapor pressure at temperature T_0 can be calculated when the moisture concentration and the initial void volume fraction are known.

The vapor pressure at temperature T for case 1 can then be obtained from equation (10) with the reference state (p_r, f_r, T_r, C_r) to be substituted by (p_0, f_0, T_0, C_0), as following

$$p(T) = \frac{Tf_0C}{T_0fC_0} p_0 = \frac{C_0 p_g(T_0)}{\rho_g(T_0)f} \frac{T}{T_0} [1 - 3\alpha(T - T_0)]$$
(17)

In case 2, the moisture in the voids is in the mixed liquid/vapor phase at *current* temperature T. Therefore, the moisture must also be in the mixed liquid/vapor phase at initial T_0 . The condition for case 2 is thus as following

$$\rho(T) \ge \rho_g(T) \tag{18}$$

or by equation (4)

$$\frac{C_0}{f} [1 - 3\alpha (T - T_0)] \ge \rho_g(T) \tag{19}$$

In this case the vapor pressure maintains the saturated vapor pressure during the course of the temperature rise. Thus the vapor pressure at temperature T follows equation (7) as follows

$$p(T) = p_g(T) \tag{20}$$

Case 3 is an intermediate case between case 1 and 2, where the moisture is in the mixed liquid/vapor phase at initial T_0 , but in the single vapor phase at current T. The condition for this case can be written as

$$\rho(T_0) > \rho_g(T_0) \quad \text{and} \quad \rho(T) < \rho_g(T) \quad (21)$$

or using equation (4)

$$C_0 / f_0 > \rho_g(T_0)$$
 and $\frac{C_0}{f} [1 - 3\alpha(T - T_0)] < \rho_g(T)$

(22)

The phase transition temperature T_1 where the moisture is just fully vaporized should be determined first according to equation (6), which can be rewritten as

$$\frac{C_0}{f(T_1)} [1 - 3\alpha(T_1 - T_0)] = \rho_g(T_1)$$
(23)

Then from T_1 to temperature T the equation (10) can be used with the reference state (p_r, f_r, T_r, C_r) to be substituted by ($p(T_1), f(T_1), T_1, C(T_1)$), as follows

$$p(T) = p(T_1) \frac{T}{T_1} \frac{f(T_1)C}{fC(T_1)} = p_g(T_1) \frac{T}{T_1} \frac{f(T_1)C}{fC(T_1)}$$

$$= p_g(T_1) \frac{T}{T_1} \frac{f(T_1)}{f} \frac{1 - 3\alpha(T - T_0)}{1 - 3\alpha(T_1 - T_0)}$$
(24)

Now the equations for calculating the vapor pressure are complete, which can be summarized as follows

$$p(T) = \frac{C_0 p_g(T_0) T}{\rho_g(T_0) f T_0} [1 - 3\alpha(T - T_0)]$$
(25)
Case 2: when $\frac{C_0}{f} [1 - 3\alpha(T - T_0)] \ge \rho_g(T)$
 $p(T) = p_g(T)$ (26)

Case 3: when $C_0 / f_0 > \rho_g(T_0)$, and

 $\frac{C_0}{f} [1 - 3\alpha (T - T_0)] < \rho_g(T)$

Case 1: when $C / f \leq \alpha (T)$

$$p(T) = p_g(T_1) \frac{T}{T_1} \frac{f(T_1)}{f} \frac{1 - 3\alpha(T - T_0)}{1 - 3\alpha(T_1 - T_0)}$$
(27)

where T_1 is determined by equation (23).

The above model includes an unknown f, the current void volume fraction. Obviously, the vapor pressure is dependent on the void deformation behaviors, and should be solved together with the governing equations of deformation.

Let's investigate the magnitude of vapor pressure for case 1, where the moisture is in single-vapor phase at Assuming that the preconditioning preconditioning. temperature T_0 is 85°C, the *maximum* vapor pressure allowed in voids at T_0 is the saturated vapor pressure $p_g(T_0=85^\circ\text{C}) =$ 5.27e-2 MPa. The vapor pressure at reflow temperature T=220°C is plotted as function of the current void volume fraction f in Fig. 3, by using equation (25) (α =200ppm/°C, $f_0=0.03$). The vapor pressure decreases with the current void volume fraction. The pressure may be lower than the initial vapor pressure of T_0 when the void becomes large. The maximum vapor pressure developed at 220°C is 7.92e-2 MPa, when the void does not grow $(f=f_0)$. The results imply that the vapor pressure for case 1 is substantially low such that it has almost negligible effect on the void growth.

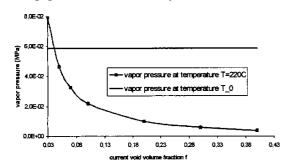


Fig.3 Vapor pressure p at 220°C versus the current void volume fraction f by equation (25) for case 1, with $f_0=0.03$, $\alpha=200$ ppm/°C, $T_0=85$ °C, and $p_0=p_{0max}=p_g(85$ °C) = 5.27e-2 MPa.

Consider the case 2 where the moisture is not fully vaporized at reflow temperature *T*. In this case the vapor pressure is the saturated vapor pressure, i.e., $p=p_{\rm g}(T=220^{\circ}{\rm C})=2.32$ MPa.

Questions remain that how to measure the initial void volume fraction f_0 . An approximate method in estimating the initial void volume fraction was proposed [2] by using the moisture absorption test. From equation (4), when moisture absorption is saturated, the initial void volume fraction is given by

$$f_0 = \frac{C_{\text{sat}}}{\rho} \tag{28}$$

Given the fact that the moisture condenses mostly into the liquid form and the water liquid density is 1.0 g/cm^3 , f_0 can be estimated from

$$f_0 \approx C_{\rm sat} \Big|_{100^{\circ}C/100RH} \tag{29}$$

Equation (29) provides a simple way to predict the approximate magnitude of the voids fraction existing in

polymer materials using the moisture property data given by Galloway et [7]. It shows that the initial void volume fraction is usually between 0.01 and 0.05.

Equation (12) can be simplified as $C \approx C_0$ when the thermal expansion is much smaller than 1. Equations (25)-(27) can then be simplified as following,

Case 1: when $C_0 / f_0 \leq \rho_g(T_0)$,

$$p(T) = \frac{C_0 p_g(T_0) T}{\rho_g(T_0) f T_0}$$
Case 2: when $\frac{C_0}{f} \ge \rho_g(T)$
(30)

$$p(T) = p_g(T) \tag{31}$$

Case 3: when
$$C_0 / f_0 > \rho_g(T_0)$$
, and $\frac{C_0}{f} < \rho_g(T)$

$$p(T) = p_g(T_1) \frac{T}{T_1} \frac{f(T_1)}{f}$$
(32)

3 Single Void Behavior: Unstable Growth Subjected to Thermal Stress and Internal Vapor Pressure in a Non-Hookean Media

As mentioned before, the above vapor pressure model should be used together with the equations of deformation and constitutive relations to investigate material behaviors during soldering. For the purpose of analysis a spherical volume of material containing a (concentric) spherically shaped micro-void as depicted in Fig. 4 is considered. The material is considered incompressible. The inner radial surface is subjected to internal vapor pressure, induced by the moisture inside. A radial stress σ^T is applied to outer radius to represent the thermal stress as function of temperature rise. The neo-Hookean model is introduced to describe the deformation behavior of rubber-like material. The stored energy function can be written as follows:

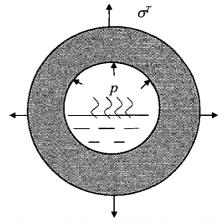


Fig.4 A micro-mechanics model of a singe void in a finite matrix in current configuration

$$W = \frac{\mu}{2} (\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3), \ \lambda_1 \lambda_2 \lambda_3 = 1$$
(33)

where μ is the shear modulus and λ_{I} are the principal stretches. It can be seen that the shear modulus is the only material property introduced in this stress-strain relation. Guo and Cheng [8] established the equilibrium solution of a spherically symmetric cell in current configuration, which can be expressed explicitly in terms of the initial and current void volume fractions f_0 and f through:

$$\frac{\sigma^{T}(T) + p(f_{0}, f, C_{0}, T, T_{0})}{\mu} = 2(\frac{1-f}{1-f_{0}})^{1/3} + \frac{1}{2}(\frac{1-f}{1-f_{0}})^{4/3} - 2(\frac{f_{0}}{f}\frac{1-f}{1-f_{0}})^{1/3} - \frac{1}{2}(\frac{f_{0}}{f}\frac{1-f}{1-f_{0}})^{4/3}$$
(34)

Equation (34) displays a nonlinear and non-monotonic relation between the applied stress (the sum of thermal stress and vapor pressure) and the void volume fraction f. This applied stress (relative to the shear modulus) versus the evolution of the void volume fraction f is shown in Fig. 5. The unstable void growth takes place when the peak value (of thermal stress + vapor pressure) is reached.

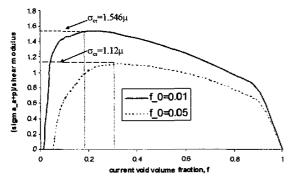


Fig. 5 The sum of thermal stress and vapor pressure applied to a cavity in a finite neo-Hookean rubber-like matrix versus the evolution of the void volume fraction f ($f_0=0.01$ and 0.05).

It is noted that using the neo-Hookean model according to equation (34), the critical stress is of the order of (1.1-1.6 times) the shear modulus μ . Assuming that $\mu = -E/3$, where at reflow temperature 220°C, a typical Young's modulus E=-500 MPa, the critical stress is of order of magnitude 165-260 MPa. The saturated vapor pressure of 2.32MPa at 220°C thus is very small compared to the critical stress (165-260 MPa) obtained for the rubber model.

From this observation it can be directly explained that the void unstable-growth was never observed in bulk material. Although the moisture exists and is evaporated anywhere in polymer materials when the entire package is exposed to the reflow temperature at 220°C, the rupture of the bulk material prior to interface delamination has never been found. This means that above model applies to the void behaviors in bulk. In the following section, the model will be extended to investigate the void behaviors at interfaces.

4 Void Behavior at Interface

The void behavior at the interface is different from that within the bulk. The void growth at the interface is not only controlled by the total stress but also the interface strength. Fig. 6 sketches the void behaviors at the interface, in which three stages are involved. At the beginning, the void at the interface has an initial void volume fraction f_0 , in which a certain amount of moisture is condensed into liquid. With the increase of the temperature, thermal stress and vapor pressure are developed and subjected to the void. The void will reach the equilibrium at the void volume fraction f_1 . Stage 1 show no difference with behaviors of voids in bulk and the stresslevel is much less than the critical stress at which the void will 'burst'. However, due to the fact that the interfacial strength is weaken by the moisture intake at high temperature, the void will continue to grow, as shown in stage 2 of Fig. 6. The new equilibrium will be reached at the void volume fraction f_2 . At this new equilibrium position, the problem can be treated as the equilibrium for a void with the initial volume void fraction $(f_0+f_2-f_1)$. If the applied stress reaches the critical stress with $(f_0+f_2-f_1)$, the void growth becomes unstable (3rd stage). Otherwise, the void growth will stop here and no further delamination is formed.

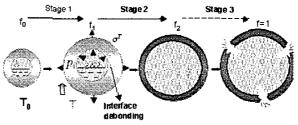


Fig. 6 Schematic description of the void behaviors at interface. Three stages are involved. Stage 1 describes the deformation during the temperature rise due to the vapor and thermal stresses. Stage 2 is the void-growth stage due to the debonding of the interface under certain stresses with the effects of the moisture intake at certain temperature. Stage 3 describes the unstable void-growth.

The void behavior at stage 2 is related to the interface properties. A general relationship between the void-growth and the moisture contents and the temperature may be postulated as following form

$$\dot{f} = kCe^{-\frac{Q}{RT}}\dot{T}$$
(35)

where C is the moisture concentration and T the temperature, R is the universal gas constant. K and Q are interface constants to be determined. It can be seen that the rate of void-growth is propertional to moisture concentration C and temperature T. Some materials exhibit excellent resistance to moisture absorption with low C, while other materials show interface strengths being quite sensitive to moisture absorption with high k. There is no direct correlation between the amount of moisture absorbed and the void-growth at interface since different materials have different k. Some failures may occur for materials with minor moisture absorption (low C), but the material has very high k. Some other materials do not fail, even with major moisture absorption (very high C), due to the excellent resistance of interface strength at high moisture concentration and high temperature (very low k). However, for *same* material the correlation between the delamination and the moisture absorption is direct and obvious. Therefore, equation (35) is a general form to describe the void behavior on interface.

The exact determination of the material properties such as k is challenging. Instead of determing equation (35), in the following, equation (34) will be applied to see how much void growth in stage 2 will lead the void grow unstablly. Let assume that the initial void volume fraction is 0.01. At the beginning the void will deform along the solid line shown in Fig. 7. Then void growth enters second stage, in which the stress-level does not change but void grows following equation (35). This stage is shown in Fig. 7 as dotted line, which will intersect with another equilibirum curve. The void will not grow further if stress-level is still below the critical stress. Otherwise, like case 2 shown in Fig. 7, the delamination will take place.

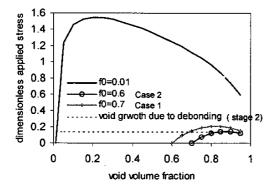


Fig. 7 void growth at interfaces

3 Discussions

The micro-mechanics analysis based on the single-void model study as discussed above, reveals some fundamental features associated with the failure mechanism for porous material such as the unstable growth of voids. How to link the results of the single void behavior to descriptions of material behavior in a macroscopic sense therefore becomes one of the critical issues. Homogenization processes can be applied for this purpose. There are several theories to establish the relationships between the microscopic and macroscopic variables [9,10]. For a porous material, the void volume fraction f is treated as a *field* variable: a damage parameter to represent the local material behavior. f=1 at a particular (continuum) point implies that delamination takes place at this 'point'. The evolution equation is required for the void volume fraction f. For homogeneous material in bulk, the growth rate can be written as [10],

$$f = f_{growth} + f_{nucleation} \tag{36}$$

$$\hat{f}_{\text{growth}} = (1 - f)\hat{E}_{kk} \tag{37}$$

$$\dot{f}_{nucleation} = A\dot{\sigma}_e + B\dot{\Sigma}_m \tag{38}$$

At interface, the impact of interface on void growth should be included

$$f = f_{growth} + f_{nucleation} + f_{debonding}$$
(39)

$$\dot{f}_{\text{growth}} = (1 - f)\dot{E}_{kk} \tag{40}$$

$$\dot{f}_{nucleation} = A\dot{\sigma}_e + B\dot{\Sigma}_m \tag{41}$$

$$\dot{f}_{\text{debonding}} = kCe^{\frac{V}{RT}}\dot{T}$$
 (42)

4 Conclusion

This paper present analytical solutions for void behavior at different stages, in bulk and at interface, based on the largedeformation theory. Mechanism of the interfacial void evolution is postulated. By taking the interface strength as function of process (moisture and temperature), the allowable critical stress for the void collapse at interface is much lower than that in bulk. Our results show that the vapor pressure is not only responsible for the increasing of interfacial stresses, but also for the decreasing of interface strength. The model also explains that the interface delamination will unlikely take place without moisture absorption, even though the temperature is increased at a higher level than the soldering temperature. The present study offers theoretical support for temperature assisted vapor-pressure-induced void initiation, growth and coalescence as the underlying mechanism of catastrophic failure.

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