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A comprehensive solution for modeling moisture induced delamination in electronic packaging during solder reflow

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ABSTRACT

Moisture induced failure is one of the major reliability concerns in electronic packaging. This research provides a comprehensive solution for modeling the moisture induced delamination in electronic packaging during solder reflow. Existing finite element approaches of studying the moisture and vapor pressure induced package delamination issue were discussed, reviewed, summarized and integrated into a systematic approach. This study covered multiple related topics, including diffusion modeling techniques under dynamic thermal loading conditions, fracture mechanics modeling methods for bi-material cracks, and methodologies of applying integrated hygro-thermal-vapor loading conditions. A novel analogy was proposed for applying the combined hygro-thermal-vapor loading in modeling the moisture induced package delamination, which could reduce the users' effort in dealing with the multiple-loading boundary conditions in the fracture mechanics finite element simulation. In the end, the comprehensive finite element approach introduced in this study was implemented to model the moisture induced delamination in a stacked die package during solder reflow.

1. Introduction

Microelectronic packaging is a multi-material system in which the polymeric materials play important roles. Typical polymeric materials such as epoxy molding compound, die attach adhesive, underfill, polyimide and solder resist are widely used in IC (Integrated Circuit) packages like QFN, PBGA, Flip-Chip and WLCSP, etc. Different from the inorganic packaging materials such as silicon, metal and ceramic, polymers have a special characteristic that they are moisture-permeable. Similar as temperature, moisture is one of the major reliability concerns that can pose a significant threat to the integrity and reliability of electronic packaging.

Moisture can affect the reliability of electronic packaging in various perspectives. From an electro-chemical perspective, moisture can result in the change of electrical characteristics (e.g. dielectric loss) of packaging materials, lead to corrosion and accelerate electromigration, which can affect the long-term reliability of semiconductor packages [1,2]. From a mechanical perspective, the effects of moisture on the packaging reliability can be mainly divided into three categories. Firstly, upon moisture absorption, polymer will have volumetric expansion which is the so-called hygroscopic swelling. In semiconductor packaging, the inorganic materials such as silicon and metal are impervious to moisture, while polymer materials are prone to absorbing moisture. Besides, polymeric materials swell at different rates. These two facts lead to a mismatch of hygroscopic swelling in packaging, which causes the swelling induced package stress in addition to the CTE (coefficient of thermal expansion) mismatch induced stress [3]. Secondly, moisture will alter the mechanical properties of polymers including glass transition temperature, elastic modulus, viscoelastic behavior and adhesion strength, which makes the IC packaging more vulnerable to cracking or delamination especially at high temperature [4]. Finally, the absorbed moisture in polymers can convert into the vapor steam upon heating, which may cause the delamination or cracking in the package [5]. If plastic IC packages are exposed to humid conditions during manufacturing, transportation and storage before the surface mount process, moisture will be absorbed by the polymer materials in the package. At the subsequent surface mount process, the package experiences a rapid heating process and the temperature goes up quickly within several minutes. The absorbed moisture turns into vapor steam and builds up several atmospheres' pressure inside the package. The high vapor pressure can trigger the inherent manufacturing defects and cause the package to deform, delaminate and crack, which can eventually lead to the “pop-corn failure” [6].

Analyzing the moisture-induced diffusion, deformation and delamination is essential for ensuring the integrity and reliability of microelectronic packaging subjected to temperature/humidity changes during the production, testing, storage and usage. Numerous efforts have been made to study the moisture related package reliability issues using both experimental and numerical methods. Among those studies, experimental methods were usually employed to characterize the moisture related material properties including moisture diffusion coefficient, saturated moisture concentration, and coefficient of

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hygroscopic swelling [7–10]. However, existing experimental methods have limitations and they are difficult to be applied in measuring parameters such as local moisture concentration, vapor pressure and hygroscopic stress, which are essential for understanding the moisture induced delamination or cracking. Under such condition, numerical methods using finite element analysis (FEA) were commonly adopted. In terms of finite element based moisture study, prior arts were mainly focused on four different topics, (1) moisture diffusion analysis [11,12]; (2) vapor pressure analysis [13]; (3) hygroscopic swelling caused deformation and stress analysis [14,15]; and (4) moisture induced delamination analysis [16,17]. Many researches were focused on topics (1, 2) and (3), while only a few efforts have been made to research the moisture induced delamination issue under the complex hygro-thermal-vapor boundary conditions such as solder reflow. Moreover, a comprehensive finite element simulation approach for modeling the moisture induced delamination in IC packaging during solder reflow was rarely seen in prior work.

The main focus of this research is to establish a systematic approach for simulating the moisture induced delamination in electronic packaging under solder reflow process. Below topics were reviewed and discussed, including simulating moisture diffusion under solder reflow, applying boundary conditions of integrated hygro-thermal-vapor loading, and modeling bi-material interfacial delamination. Delamination behavior of a moisture-preconditioned stacked die package under the solder reflow process was investigated by the finite element analysis based on linear elastic fracture mechanics.

2. Theory and methodology

2.1. Moisture diffusion modeling

The commonly-used theory for modeling moisture diffusion in polymers is the Fick's second law, which assumes that the moisture concentration gradient drives diffusion flux. The governing equation of moisture diffusion in an isotropic polymeric material is given by

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{1}$$

where t is time, C is the moisture concentration, D is the diffusivity, and x, y, z are Cartesian coordinates.

Eq. (1) is suitable for modeling moisture diffusion in a homogeneous material. For a multilateral system like microelectronic packaging, the moisture concentration distribution is not continuous across the bi-material interface (e.g. underfill/substrate interface, molding compound/substrate interface), which is not similar as the temperature distribution. The main reason causing the discontinuity is that dissimilar materials have different moisture absorption capacities. To analyze the moisture diffusion behavior in a bi-material with finite element method, the moisture concentration discontinuity issue has to be resolved.

The normalization method has been adopted as a common practice to tackle the above-mentioned concentration discontinuity problem. The interfacial moisture concentration discontinuity can be removed by replacing the moisture concentration C with a normalized field variable w, named "wetness" or "fractional saturation" [18]. The normalized concentration w is continuous across the shared boundary of adjacent materials and it can be expressed with the following equation:

$$w = \frac{C}{C_{sat}} \tag{2}$$

where C_{sat} is the saturated moisture concentration that defines the maximum moisture uptake of polymer under a given temperature-humidity condition. Then, the diffusion governing equation can be reformulated using the newly-defined dimensionless parameter "w" as

$$\frac{\partial w}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) \tag{3}$$

The commonly used normalization method described in Eq. (3) is valid only when C_{sat} is a constant. It has been revealed by experimental observation that C_{sat} is a function of temperature [19]. It indicates that, under a temperature-changing condition such as solder reflow, C_{sat} is no longer an invariant. Because the temperature is changing with time during reflow, the C_{sat} also varies with time. Under such condition, the diffusion governing equation would become

$$\frac{\partial w}{\partial t} + \frac{w}{C_{sat}}\frac{\partial C_{sat}}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) \tag{4}$$

It should be noticed that, there is an additional term in Eq. (4) compared to Eq. (3). In a temperature-varying condition, directly inputting C_{sat} as a function of temperature in some commercial finite element software (ANSYS version earlier than 17, ABAQUS and COMSOL) will yield erroneous results [20], because the second term on the left-hand side in Eq. (4) is not considered in the software algorithm during the solving process. Various methods have been proposed by researchers to solve this problem.

Xie [21] introduced the "direct concentration approach (DCA)", in which the constraint equation was used to establish the concentration relationship at the shared material boundary in a bi-material system. However, it has been observed that the diffusion flux across the bi-material interface is discontinuous when applying the direct concentration approach in diffusion simulation, which means the law of mass conservation is violated [22]. Jang [23] developed the "advanced normalization method" in which a constant term M was utilized to define the normalized variable to replace the usage of C_{sat}. However, this method is not universally applicable because it requires the equivalence of activation energies of solubility for two adjacent polymer materials. Essentially, the "advanced normalization method" is the equivalent to the traditional normalization method which treats C_{sat} as a constant term during normalization. The peridynamics theory was applied by Oterkus [24] in the diffusion finite element modeling to overcome the moisture discontinuity problem. Unlike the classic continuum mechanics theory which uses partial differential equations, the peridynamic theory is based on the integral-formed governing equations. However, directly combining peridynamics theory with finite element method will neglect the fact of moisture concentration discontinuity at material interface, which means it cannot correctly describe the physics of moisture diffusion if this method is directly implemented. The normalized concentration is still required when using this theory, therefore the "peridynamic wetness approach" was proposed later [25]. Nonetheless, utilizing "peridynamic wetness approach" cannot directly solve the diffusion problem with a varying C_{sat}, more other efforts are still needed to deal with the extra term in Eq. (4). Using this approach will require tremendous amount of effort in meshing and solving especially when dealing with complex geometric structure, which limits its field of application. Since the release of ANSYS version 17 [26], the problem in bi-material moisture diffusion with a temperature-dependent C_{sat} is directly solved by including the extra term that describes the temperature-dependency of C_{sat} in the software algorithm. However, this implementation can only be used in the couple-field element (e.g. PLANE 223) instead of the diffusion element (e.g. PLANE 238). Besides, users need to be very careful when choosing the proper time step size, because a relatively large time step size may lead to inaccurate results when using ANSYS 17 or later version [27].

In this study, an alternative approach called "internal source technique" was used to deal with the moisture diffusion with a temperature-dependent C_{sat}. The "internal source technique" was first proposed by Wong [28], and later the accuracy of this technique was examined by the author in [27]. In this diffusion modeling technique, the internal source is applied as a boundary condition in the commercial finite element software to compensate for the extra term in Eq. (4).

The diffusion governing equation with an internal source term can be written as

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) + r \tag{5}$$

where r is defined as the diffusing substance generation rate per unit volume. Defining $C = wC_{sat}$ and Eq. (5) can be reformulated as

$$\frac{\partial w}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) + \frac{r}{C_{sat}} \tag{6}$$

Moving the second term from left-hand side to right-hand side, Eq. (4) becomes

$$\frac{\partial w}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) - \frac{w}{C_{sat}}\frac{\partial C_{sat}}{\partial t} \tag{7}$$

If Eqs. (6) and (7) are set to be equivalent, then the internal source term r can be calculated as

$$r = -w\frac{\partial C_{sat}}{\partial t} \tag{8}$$

The term r in Eq. (8) can be applied as an internal source boundary condition in FEA software to substitute the last term on right-hand side in Eq. (7). In this way, the omitted term in commercial finite element software can be compensated during calculation. If the normalized concentration field w_{t_i} at time t_i is given, and the target is to obtain $w_{t_i+\Delta t}$ which is the normalized concentration field at time $t_i + \Delta t$. At the time step $t_i + \Delta t$, the time dependency of C_{sat} can be estimated as the finite difference form with backward Euler method as

$$r = -w\frac{\partial C_{sat}}{\partial t} = -w_{t_i+\Delta t}\frac{C_{sat}^{t_i+\Delta t} - C_{sat}^{t_i}}{\Delta t} = w_{t_i+\Delta t}\frac{C_{sat}^{t_i} - C_{sat}^{t_i+\Delta t}}{\Delta t} \tag{9}$$

where ${C_{sat}}^{t_i}$ is the saturated moisture concentration at t_i and ${C_{sat}}^{t_i+\Delta t}$ is the saturated moisture concentration at $t_i + \Delta t$. It should be noticed that, the normalized concentration field $w_{t_i+\Delta t}$ in Eq. (9) is not determined yet and cannot be utilized to calculate the internal source term r. The moisture concentration does not have noticeable change during consecutive time incremental steps if the time step Δt is small, because the moisture diffusion process is relatively slow. Based on the law of mass conservation, relationship can be built between $w_{t_i+\Delta t}$ and w_{t_i} as

$$w_{t_i+\Delta t} = \frac{w_{t_i} C_{sat}^{t_i}}{C_{sat}^{t_i+\Delta t}} \tag{10}$$

Substituting Eq. (10) into Eq. (9), the internal source term r can be expressed as

$$r = \frac{w_{t_i} C_{sat}^{t_i}}{C_{sat}^{t_i+\Delta t}}\frac{C_{sat}^{t_i} - C_{sat}^{t_i+\Delta t}}{\Delta t} \tag{11}$$

To implement the internal source technique in diffusion modeling using the finite element analysis, C_{sat} should be input as a temperature-dependent material property first. If a temperature-dependent C_{sat} is not supported by the FEA software, users can update the C_{sat} material property at each time step. The normalized concentration field at time t_i needs to be calculated in order to determine the internal source term r_i which will be applied as an internal source boundary condition at time $t_i + \Delta t$. Thus, the normalized concentration field $t_i + \Delta t$ will be obtained and can be used to determine r_{i+1} in the following time step (Fig. 1).

The internal source technique is a promising method because it provides a universal solution to model diffusion problems in a multi-material system under dynamic thermal loading conditions without the need to assume the temperature-independence of C_{sat}. Also it is a practical methodology that can be applied in various commercial finite element software that do not support the new diffusion function

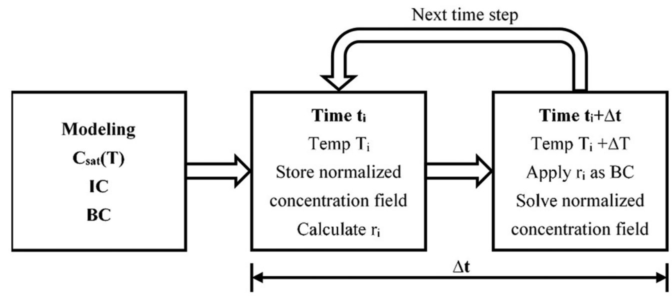

Fig. 1. Implementation of the internal source approach.

introduced in ANSYS 17. In this study, the internal source technique was used to model the moisture diffusion in the electronic package during solder reflow.

2.2. Interfacial delamination in bi-material

An electronic package usually consists of several different materials such as silicon, metal and polymer. One common failure mode of packaging is the interfacial delamination. When the local stress is sufficiently large, cracks are likely to be initialized at the material interfaces in the electronic package. Manufacturing defects or voids can also become potential risk sites for delamination occurrence. Linear elastic fracture mechanics is widely adopted to analyze the delamination behavior of bi-material interfacial cracks. There are three commonly used approaches that can determine fracture parameters (e.g. stress intensity factor, strain energy release rate, etc.) for bi-material interfacial cracks. They are crack tip opening displacement method (CTOD), virtual crack closure technique (VCCT) and J-integral.

The crack tip opening displacement (CTOD) method is a classic way to calculate the fracture parameters for an interfacial crack in a bi-material system (Fig. 2). This method can be used to determine the stress intensity factors and strain energy release rate based on the values of displacement change near the crack tip [29]. However, CTOD is a not built-in feature in commercial finite element software such as ANSYS. It would be inconvenient for users to implement this method, because the raw displacement data has to be extracted from the simulation results manually to determine fracture parameters based on the CTOD formulas.

J-integral is a widely used domain integral method in fracture mechanics. It is a path integral along an arbitrary curve over a scalar field and one of its primary characteristic is the path-independence. J-integral can be used to analyze interfacial cracks in nonhomogeneous structures and can be easily implemented in commercial finite element software such as ANSYS [30]. Although J-integral under different fracture modes can be determined by analytical methods [31], the mode separation is not supported in post-processing features of commercial finite element software such as ANSYS.

The virtual crack closure technique (VCCT) was initially proposed by Rybicki and Kanninen [32], and it is one of the favorite numerical fracture mechanics methods to calculate the strain energy release rates for enabling the mode separation required in the mixed mode fracture

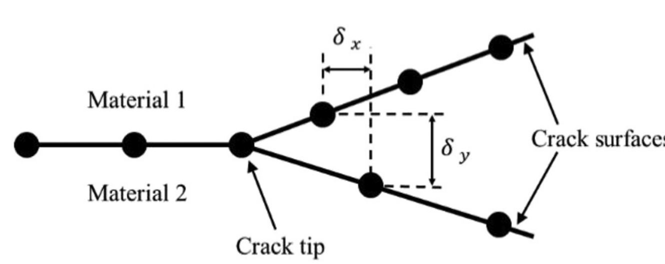

Fig. 2. Crack tip opening displacement (CTOD).

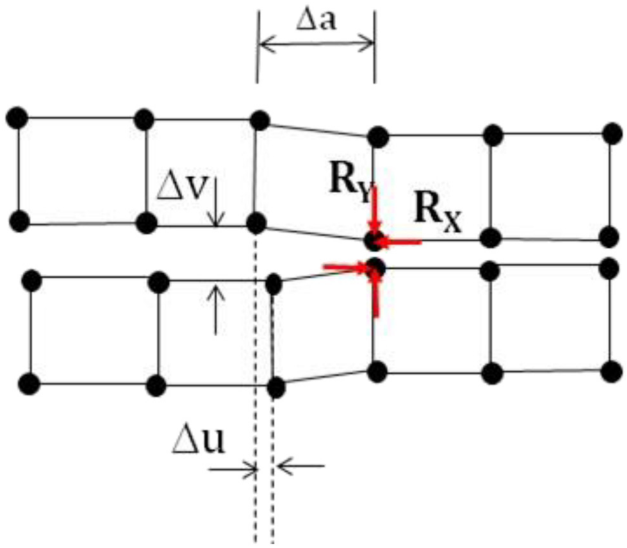

Fig. 3. Mesh used in virtual crack closure technique [26].

criterion. This well-established method is based on Irwin's crack closure integral with the assumption that, the amount of energy released when the crack is extended by an infinitesimal distance is identical to the energy required to close the crack to its original length. In a two-dimensional domain (Fig. 3), the strain energy release rate components of Mode I (G_I) and Mode II (G_{II}) can be determined as

$$G_I = -\frac{1}{2\Delta a} R_Y \Delta v \tag{12}$$

$$G_{II} = -\frac{1}{2\Delta a} R_X \Delta u \tag{13}$$

where Δa is a small length of crack extension, R_x and R_y are the nodal reaction forces at the crack-tip node in x (shearing mode) and y (opening) directions, respectively, Δu and Δv are the nodal displacements at the nodes with a small distance ahead of the crack tip along the x (shearing mode) and y (opening mode) directions, respectively. The total strain energy release rate G_{tot} can be determined based on G_I and G_{II} as

$$G_{tot} = G_I + G_{II} \tag{14}$$

The VCCT method can be used with the conventional non-singular and linear element to obtain accurate strain energy release rate results in the finite element analysis. To get relatively accurate results, the four elements adjacent to the crack tip are suggested to have similar mesh size, and the virtual crack extension length Δa should be sufficiently small. In this article, the VCCT method is adopted in the finite element modeling.

2.3. Integrated hygro-thermal-vapor loading

The moisturized package has the potential risk of delamination induced failure during solder reflow process, because thermal expansion, hygroscopic swelling and vapor pressure contribute at the same time. To analyze such a multiphysics phenomenon, all above three different effects need to be considered in the simulation.

Microelectronic assemblies consist of materials that have a wide range of CTE (coefficient of thermal expansion), and the CTE mismatch among dissimilar materials is the major cause of thermo-mechanical failures of IC packaging. The stress intensity factor due to thermal expansion K_t can be interpreted as

$$K_t = K_{I,t} + iK_{II,t} \tag{15}$$

where $K_{I,t}$ and $K_{II,t}$ are the stress intensity factors of mode I and II due to thermal expansion, respectively.

Volumetric expansion occurs when polymeric material absorbs moisture, which is the well-known phenomenon named hygroscopic swelling. Similar to the CTE mismatch, the CHS (coefficient of hygroscopic swelling) mismatch exists among dissimilar materials in the package after moisture absorption, which is the major cause of hygro-mechanical failures. The stress intensity factor due to hygroscopic swelling K_h can be interpreted as

$$K_h = K_{I,h} + iK_{II,h} \tag{16}$$

where $K_{I,h}$ and $K_{II,h}$ are the stress intensity factors of mode I and II due to hygroscopic swelling, respectively.

Polymers contain nano pores and voids where moisture can be trapped. During rapid heating, moisture will vaporize and exert pressure on the inner surface of the pores, voids or small cracks in the packaging. The stress intensity factor due to vapor pressure K_P can be interpreted as

$$K_p = K_{I,p} + iK_{II,p} \tag{17}$$

where $K_{I,p}$ and $K_{II,p}$ are the stress intensity factors of mode I and II due to vapor pressure, respectively.

Once the individual stress intensity factors are determined, the stress intensity factor K_{tot} caused by the combined effect of thermal expansion, hygroscopic swelling and vapor pressure can be calculated based on the principle of superposition as [33].

$$K_{tot} = (K_{I,t} + K_{I,h} + K_{I,p}) + i(K_{II,t} + K_{II,h} + K_{II,p}) \tag{18}$$

The combined strain energy release rate G_{tot} can be determined as [33].

$$G_{tot} = \frac{(K_{I,t} + K_{I,h} + K_{I,p})^2 + (K_{II,t} + K_{II,h} + K_{II,p})^2}{\cosh^2(\pi\varepsilon)\cdot E^*} \tag{19}$$

where E* is effective modulus and ε is oscillatory index.

The above superposition based method is a conventional way to calculate the total stress intensity factor and strain energy release rate under the combined hygro-thermal-vapor loading. This method is straightforward but inconvenient to implement, because three separate finite element analyses are needed to simulate the individual effect of thermal loading, hygro loading and vapor pressure. Moreover, K_{tot} and G_{tot} cannot be directly calculated based on effective K_t, K_h and K_p, because the stress intensity factors under different fracture modes needs to be extracted.

In fact, the three separate delamination analyses under thermal expansion, hygroscopic swelling and vapor pressure can be simplified into a single analysis [34]. To achieve the above-mentioned fracture mechanics simulation in a single run, three types of boundary conditions shall be applied simultaneously. The vapor pressure loading itself is relatively simple to apply. A surface loading with the appropriate vapor pressure value shall be exerted on the crack surface in normal direction to represent the effect of vapor pressure loading [35]. The simulation challenge arises from applying the thermal and hygroscopic loadings at the same time, because hygroscopic loading is not directly supported in the fracture mechanics simulation feature when using ANSYS.

To simultaneously apply the moisture and temperature boundary conditions, researchers have proposed different solutions. The commonly used ways for achieving integrated hygro-thermal loading are “equivalent CTE” and “equivalent temperature” methods [36,37]. As shown in Eq. (20), the hygroscopic strain ε_h is integrated into the thermal strain ε_t, so that an “equivalent CTE” or “equivalent temperature” can be calculated and applied in the finite element simulation. However, both methods have disadvantages and limitations. The “equivalent CTE” method is not applicable when the moisture concentration field is non-uniform, while the “equivalent temperature” method may generate erroneous results when temperature-dependent material properties are input in the simulation, because material

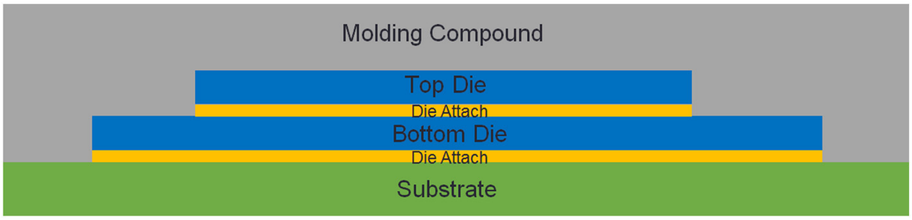

Fig. 4. Schematic of stacked die package.

properties associated with an "equivalent temperature" will be triggered in the solving process rather than the actual temperature. Therefore, both of these two methods have limited field of application.

$$\varepsilon_t + \varepsilon_h = \alpha\Delta T + \beta C = \Delta T\left(\alpha + \frac{\beta C}{\Delta T}\right) = \alpha\left(\Delta T + \frac{\beta C}{\alpha}\right) \quad (20)$$

where α is the coefficient of thermal expansion (CTE), ΔT is the temperature change, β is the coefficient of hygroscopic swelling (CHS) and C is the moisture concentration.

To mimic the effect of hygroscopic swelling, another method was developed by leveraging the user-defined swelling model in ANSYS [26,38]. The swelling strain is defined as follows:

$$\varepsilon_{sw} = r(\phi_t)^n \quad (21)$$

where ε_{sw} is the swelling strain, r is the swelling rate, n is the exponent and ϕ_t is the "fluence". The "fluence" is a body load which can be used to represent the moisture concentration field. When defining r, ϕ_t and n as β, C and 1, respectively, Eq. (21) becomes equivalent to the hygroscopic strain formula $\varepsilon_h = \beta C$. This method does not have the limitations shown in "equivalent CTE" and "equivalent temperature" methods. However, this user-defined swelling function can only be applied in the ANSYS legacy elements (e.g. PLANE 82) which do not support the advanced post-processing features if using VCCT or J-integral in the fracture mechanics simulation.

In this article, a novel approach was proposed based on the above mentioned "swelling" analogy. Besides the user-defined swelling model, a built-in swelling function is also available in ANSYS [26], which is named as "exponential swelling model". This model can be expressed as

$$\varepsilon_{sw} = C_1 + C_2\phi_t + C_3[\exp(-C_4\phi_t) - 1] \quad (22)$$

It should be noticed that, Eq. (22) can become equivalent to hygroscopic strain expression $\varepsilon_h = \beta C$, if C_1 and C_3 are set as zero, and ϕ_t and C_2 are defined as C and β, respectively. Similar as the model described in Eq. (21), the "fluence" can be interpreted as a body load in addition to the temperature in the hygro-thermal loading. Unlike above mentioned analogy in Eq. (21), this novel analogy is applicable in the latest elements (e.g. PLANE 183) which supports the convenient post-processing feature of obtaining fracture parameters such as strain energy release rate and stress intensity factor using either VCCT or J-integral. Hence, users can conveniently get the fracture parameters under the combined hygro-thermal loading boundary condition when the proposed analogy is used. Moreover, this method can be applied under temperature-dependent β and non-uniform temperature field, which makes it a universal methodology to apply the integrated hygro-thermal loading in the simulation.

3. Finite element modeling

In the present work, finite element analysis was implemented to investigate the hygro-vapor-thermo-mechanical behavior of a stacked die package during precondition. Precondition is a typical reliability testing item in JEDEC standard, which is intended to simulate the viability of packages during the surface mount process and mimic the environment of the production floor that packages may be stored in a humid environment. During precondition, the IC package would first be baked for 24 h to remove existing moisture, and then soaked under specific moisture sensitivity level (MSL) for certain amount of time. After moisture soaking, three times of reflow will be performed on the package. During solder reflow, the package undergoes rapid heating and the moisture absorbed by the package turns in to steam when the package temperature is over the water boiling temperature, which leads to a significant increase of vapor pressure. In addition to the vapor pressure, the effects of hygroscopic swelling, thermal expansion and material degradation occur simultaneously, and delamination is likely to generate inside the package.

In this finite element simulation, an integrated analysis considering thermal-hygro-vapor loading was performed to study the delamination in the stacked die package during precondition. Fig. 4 shows the geometry schematic of the stacked die package, including two silicon dies, molding compound, die attach adhesive and substrate. In this modeling, the precondition process was simplified to moisture soaking followed by one time of reflow. Moisture soaking under MSL 1 (85 °C/85% RH for 168 h) was first performed on the stacked die package. The package was then subjected to a lead-free solder reflow process with a peak temperature at 260 °C (reflow temperature profile is shown in Fig. 5). In the simulation, only the stage of heating up from room temperature (25 °C) to the peak temperature (260 °C) was considered for the reflow process, while the cooling down process was not covered.

In this study, two different types of analysis were performed – moisture diffusion analysis and fracture mechanics analysis. In the first section, the moisture absorption process during soaking was simulated using diffusion analysis. Then the moisture concentration result from the moisture absorption analysis was taken as the initial boundary condition for simulating the moisture desorption during the reflow process. In the second section, the delamination behavior of the package under the combined hygro-thermal-vapor loading was simulated using the fracture mechanics based analysis.

3.1. Moisture diffusion analysis

To analyze the moisture diffusion behavior in the package during moisture soaking and reflow, a two-dimensional (2D) diffusion analysis

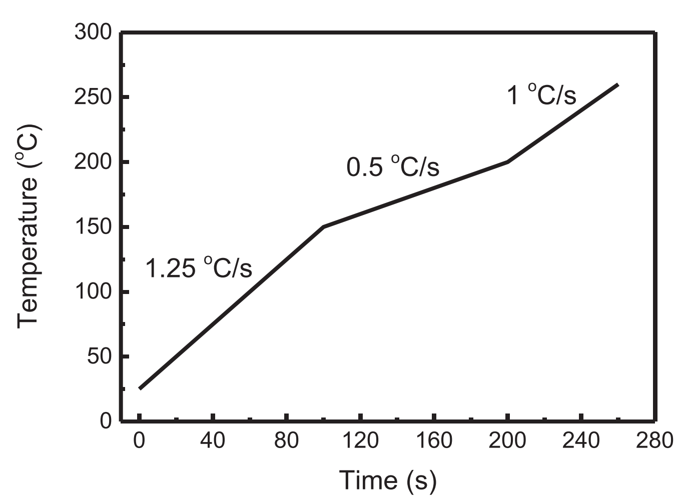

Fig. 5. Reflow temperature profile.

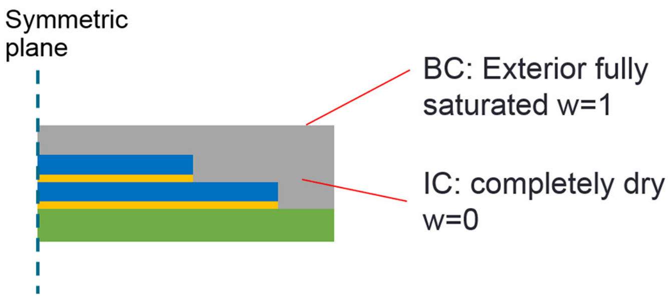

Fig. 6. Initial and boundary conditions in moisture absorption analysis.

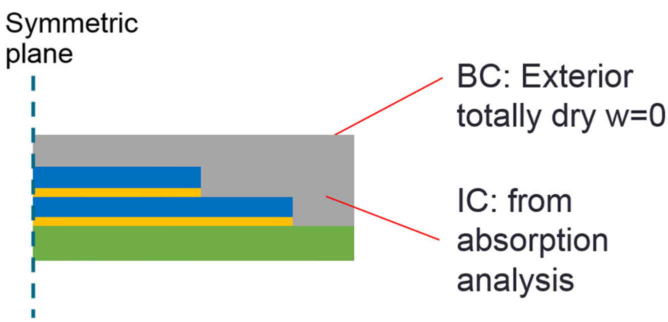

Fig. 7. Initial and boundary conditions in moisture desorption analysis.

was conducted using the commercial finite element analysis software ANSYS. It was assumed that, the molding compound, die attach and substrate absorb moisture, while the silicon die does not absorb any moisture. Only half of the package was modeled due to symmetry. At the stage of soaking, an absorption analysis under constant moisture condition (85 °C/85% RH for 168 h) was performed. The moisture concentration of exterior boundary of the package was set to be fully saturated (w = 1) and interior was set as totally dry (w = 0) during the whole 168 h soaking, and the symmetry plane was set to be diffusion flux free (shown in Fig. 6). At the stage of reflow, a moisture desorption analysis was performed. The initial condition of moisture concentration was extracted from the moisture absorption analysis while the exterior boundary was set as completely dry condition (w = 0), as shown in Fig. 7. Since the reflow process is temperature-varying and C_{sat} changes with temperature, the internal source technique was adopted to analyze the moisture desorption during solder reflow. For the temperature boundary condition, the heat transfer within the package during reflow was assumed to happen within short time due to the fact that, the package size is small so that the temperature difference within the package should be small. Therefore, the temperature field across the package can be treated as uniform at specific time. At each time step, a uniform temperature loading was applied on the whole stacked die package.

3.2. Fracture mechanics analysis

In this section, the delamination behavior of the stacked die package under combined hygro-thermal-vapor loading during solder reflow was investigated by the fracture-mechanics based finite element analysis. A two-dimensional (2D) finite element model was built in ANSYS using PLANE182 element and plane strain condition was assumed in the analysis.

Generally, the plastic IC package tends to have delamination at material interfaces that have large CTE and CHS mismatch during solder reflow. In this study, four potential delamination interfaces were considered in this simulation, they are (1) top die/die attach interface, (2) top die/molding compound interface, (3) bottom die/die attach interface, and (4) bottom die/molding compound interface. To perform the fracture mechanics based analysis, initial cracks were inserted in the model (shown in Fig. 8). The cause of initial cracks or voids in the package could be from manufacturing defects or improper processing. Large stress concentration caused by the comprehensive effect of hygro-thermal-vapor loading could also result in the crack initiation. In the local modeling of the inserted cracks, the upper and lower crack surfaces were modeled to be separate but still at coincident location. To avoid the inter-penetration between upper and lower crack surfaces, contact pairs were modeled at the crack surfaces.

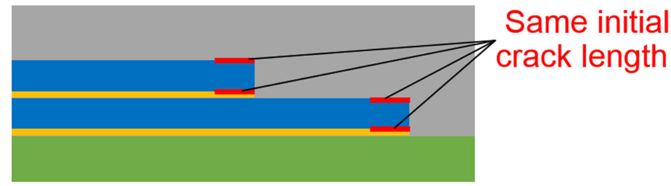

Fig. 8. Vertically distributed initial cracks at different material interfaces.

One difficulty in modeling the package delamination behavior during solder reflow is to calculate the vapor pressure inside the crack or void. Multiple theoretical models have been developed to study the evolution of vapor pressure in packaging polymers during reflow process. Generally, these vapor pressure models can be divided into two categories, Henry's law-based models [39] and micromechanics-based vapor pressure model [40,41]. Most of the models proposed so far follow ideal gas law. Because the vapor pressure model is not the focus of this paper, the author used the Henry's law based vapor pressure model which is simple to implement [39]. It is assumed that when the crack is initiated, the surrounding moisture would fill into the crack and vapor pressure exerted on the crack surfaces is proportional to the local moisture content. The vapor pressure can be determined as

$$P(T) = P_{sat}(T) \times RH \times w(T) \quad (23)$$

where $P_{sat}(T)$ is the saturated water vapor pressure at temperature T and it can be obtained from the steam table, RH is the relative humidity for the environment during moisture soaking, w(T) is the average normalized concentration around the crack at temperature T. Normal traction was applied at upper and lower crack surfaces with the calculated water vapor pressure P(T), as shown in Fig. 9.

To apply the hygroscopic swelling boundary condition during solder reflow, the moisture concentration field at each loading step was obtained from corresponding time points at moisture desorption analysis. Then, the method described in Eq. (22) was used to apply the integrated hygro-thermal loading. The reference temperature of the whole package was selected as 175 °C which is the curing temperature of the molding compound. Temperature loading following the profile in Fig. 5 was applied as a body force on the package at each time step.

4. Results and discussion

Fig. 10 plots the normalized concentration field in the stacked die

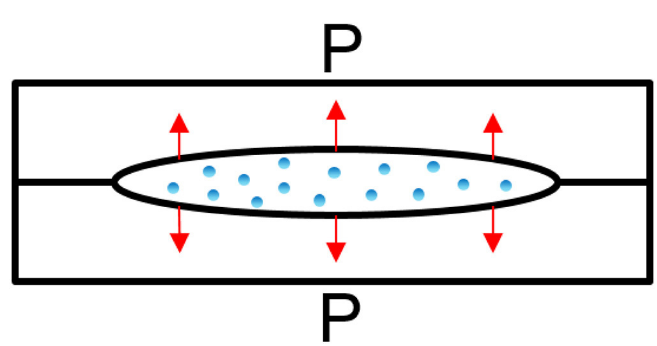

Fig. 9. Vapor pressure applied on crack surfaces.

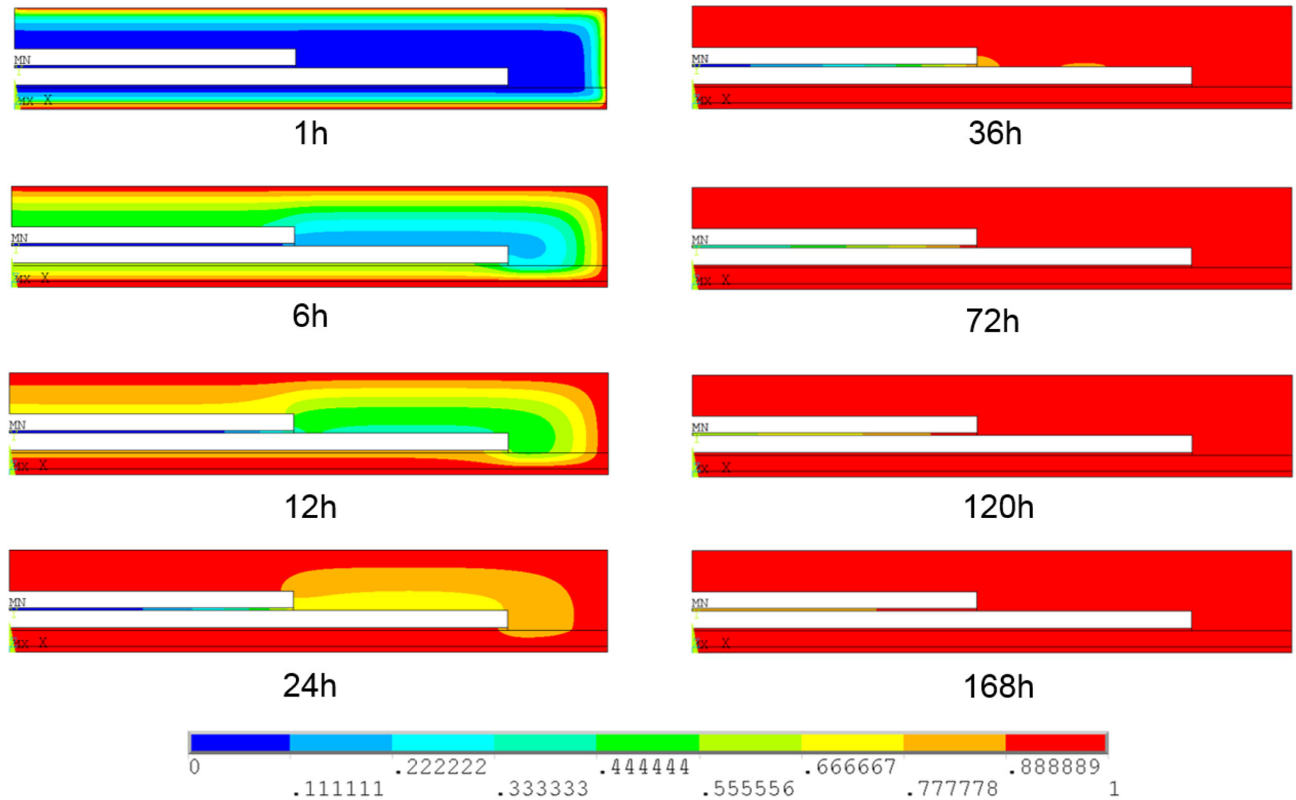

Fig. 10. Normalized moisture concentration field during soaking.

package at different time points during moisture soaking. It can be seen that, the moisture concentration continues to increase during the 168 h soaking process. The moisture diffusion happens relatively fast at the initial 24 h and becomes relatively slow at the later time. After 168 h soaking under MSL 1 (85 °C/85% RH), the stacked die package reaches a near-saturation state. The substrate, molding compound and bottom die attach are fully saturated at 168 h, while the top die attach material is not saturated. This main reason is because the die attach layer is embedded between two silicon dies that are impermeable to moisture. The diffusion path for moisture to enter into the top die attach material in vertical direction is blocked by the silicon chips, and the only path that allows moisture to diffuse into top die attach is the horizontal direction. The length of package is much larger than the thickness, therefore it requires longer time for the top die attach to get saturated.

The normalized moisture concentration field at solder reflow is shown in Fig. 11. The diffusion in the package during solder reflow is a moisture desorption process in which the moisture continues to diffuse out of package. Compared to the moisture absorption at MSL 1 which happens in a relatively long time period (168 h), the moisture desorption at reflow is a very fast process. This is due to the fact that the reflow temperature can reach much higher (up to 260 °C) than the temperature at moisture soaking (85 °C). According to the Arrhenius relationship, the higher the temperature the larger the diffusivity will be. Within 260 s, the temperature of package reach 260 °C, and there is significant amount of moisture loss in the substrate, bottom die attach and molding compound. Nonetheless, lots of moisture still remains in the interior of molding compound and the top die attach material. High vapor pressure as well as high hygroscopic stress can be induced by this high amount of residue moisture in polymeric materials. It increases the possibility of package delamination, which may pose a significant threat to the package reliability.

The total strain energy release rate under the comprehensive effect of thermal expansion, hygroscopic swelling and vapor pressure is evaluated. The relationship between the strain energy release rate and temperature for top die/die attach and bottom die/die attach interfaces is shown in Fig. 12. Fig. 13 plots the variation of the strain energy release rate versus temperature at the top die/molding compound and the bottom die/molding compound crack interfaces. It can be concluded from these two plots that, the strain energy release rate shows a nonlinear increase with temperature for both die/die attach and die/molding compound interfaces. The strain energy release rate at the bottom die/die attach crack is larger than that of the top die/die attach

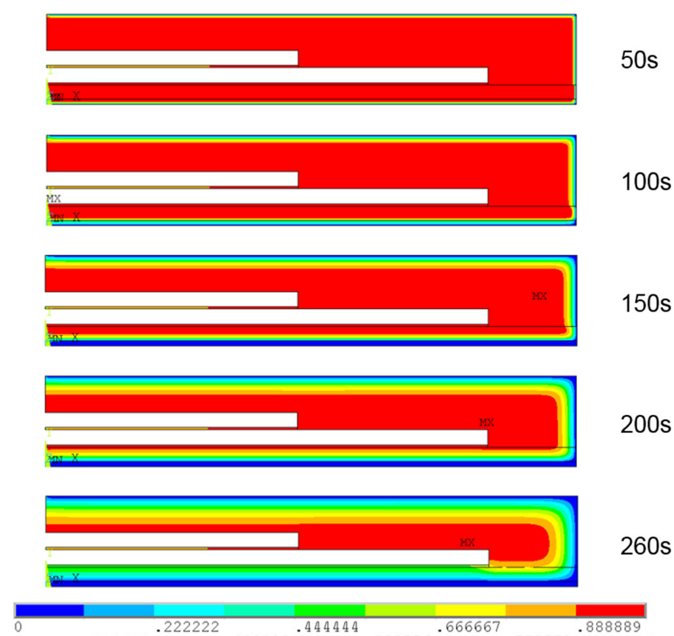

Fig. 11. Normalized moisture concentration field during reflow.

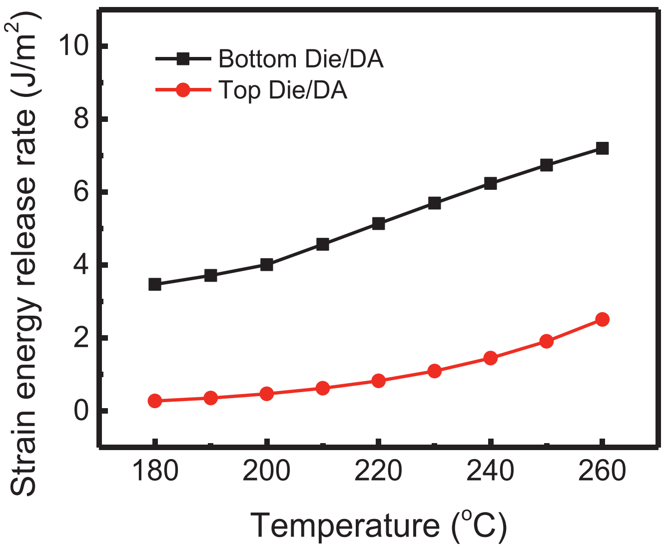

Fig. 12. Strain energy release rate under different temperatures at die/die attach interface.

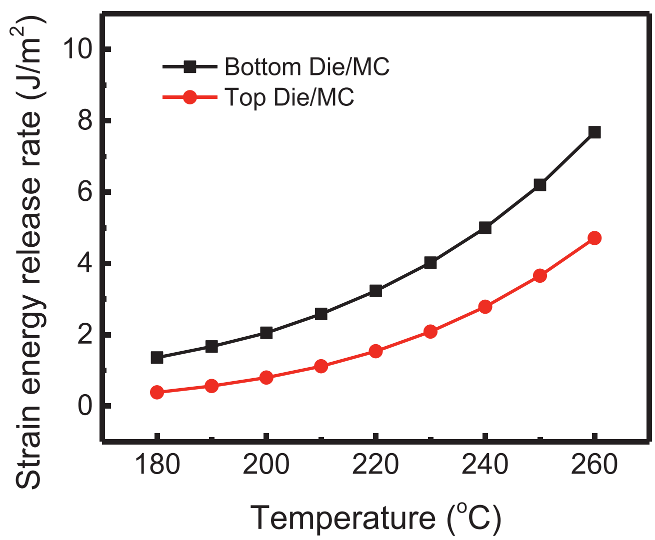

Fig. 13. Strain energy release rate under different temperatures at die/molding compound interface.

crack. Similar trend can also be found at die/molding compound interfaces, where the bottom die/molding compound interfacial crack yields larger strain energy release rate than the top die/molding compound interfacial crack. This phenomenon is generally caused by the large distance-to-neutral point (DNP) of the bottom die.

The influence of the horizontal crack position on strain energy release rate and phase angle is also investigated. As shown in Fig. 14, for each type of crack interface (bottom die/die attach or top die/molding compound), four different crack positions were considered. All initial crack lengths were assumed to be 0.2 mm. The strain energy release rate is plotted against different crack positions in Figs. 15 and 16 for bottom die/die attach and top die/molding compound interfacial cracks, respectively. As can been seen from the two figures, the strain energy release rate and phase angle increase when the crack position (distance from crack tip to package center) varies from the center to the right edge for both bottom die/die attach and top die/molding compound interfacial cracks. The values of strain energy release rate and phase angle at the edge location are much larger than those at the center location. For the die/die attach interface at bottom die, from center to edge, the phase angle changes from a value less than 45 degrees to a value larger than 45 degrees, meaning that the edge location is shear stress dominant while the center location is normal stress dominant.

Fig. 14. Horizontally distributed initial cracks at material interfaces.

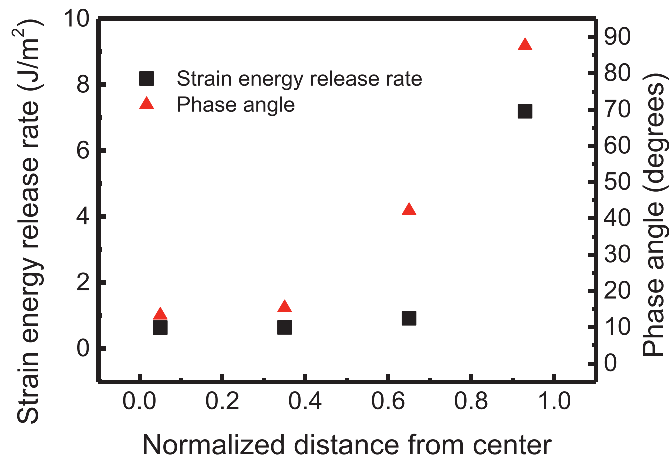

Fig. 15. Strain energy release rate and phase angle at different locations at bottom die/die attach interface.

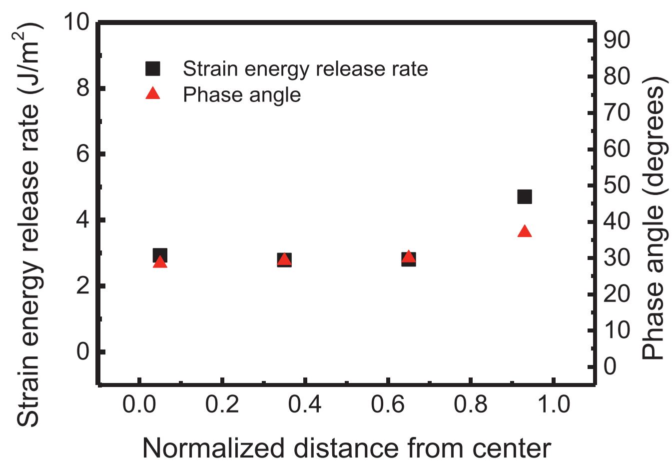

Fig. 16. Strain energy release rate and phase angle at different locations at top die/molding compound interface.

From above results, it is known that the strain energy lease rate of crack at bottom die is larger than that of top die. In this case, the initial crack is considered to occur at the edge of bottom die only. The relationship between strain energy release rate and initial crack lengths for bottom die/die attach and bottom die/molding compound interfacial cracks are plotted in Figs. 17 and 18, respectively. Five different initial crack lengths are considered. Both Figs. 17 and 18 show that the strain energy release rate increases with the crack length. The total strain energy release rate rises slowly with initial crack length at a relatively low temperature (180 °C). The growth trend of strain energy

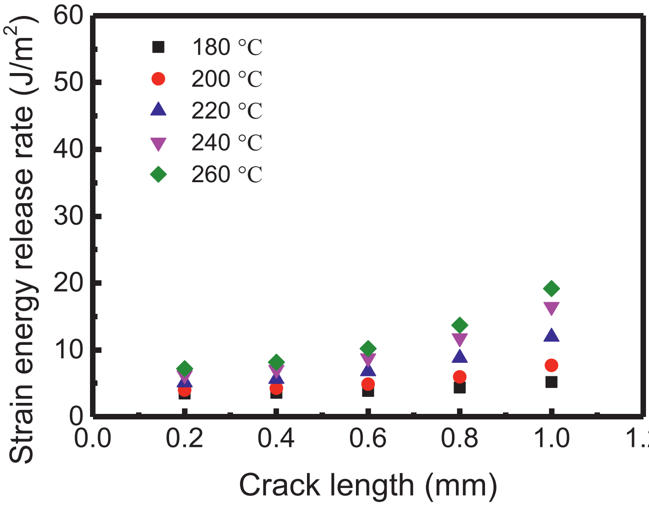

Fig. 17. Strain energy release rate with different crack lengths under different temperature at bottom die/die attach interface.

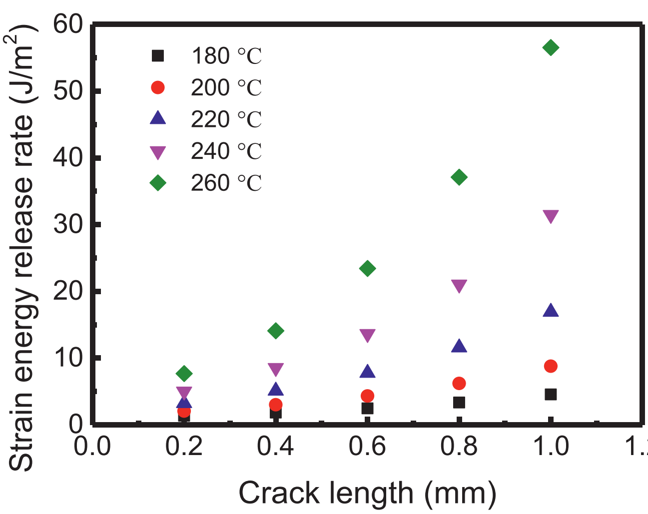

Fig. 18. Strain energy release rate with different crack lengths under different temperature at bottom die/molding compound interface.

release rate becomes more significant when the temperature reaches 260 °C. The root cause of this phenomenon is that, for a larger initial crack length, the contribution of vapor pressure becomes more important. It can also be discovered that, the growth rate of the strain energy release rate with crack length is higher for bottom die/molding compound interfacial crack when comparing to the bottom die/die attach interfacial crack.

The mode mixity (or phase angle) of the interfacial cracks are also evaluated for crack tips at both bottom die/die attach and bottom die/molding compound, which are plotted in Figs. 19 and 20, respectively. It can be seen from the two figures that, as the initial crack length grows, the phase angle decreases for both two scenarios. For the crack at die/die attach interface, the phase angle decreases first and becomes relatively stable when initial crack length is close to 1 mm. The decreasing trend of phase angle with crack length is more obvious for the cracks at bottom die/molding compound interface. For a relatively small crack length and when the temperature is close to 180 °C, a nearly pure shearing mode is shown at the crack tip, which is mainly caused by the major contribution of CHS mismatch and CTE mismatch. In contrast to the thermal and hygroscopic mismatch, the vapor pressure usually results in an opening mode of the crack. With the increase of either crack length or temperature, the influence of vapor pressure plays more

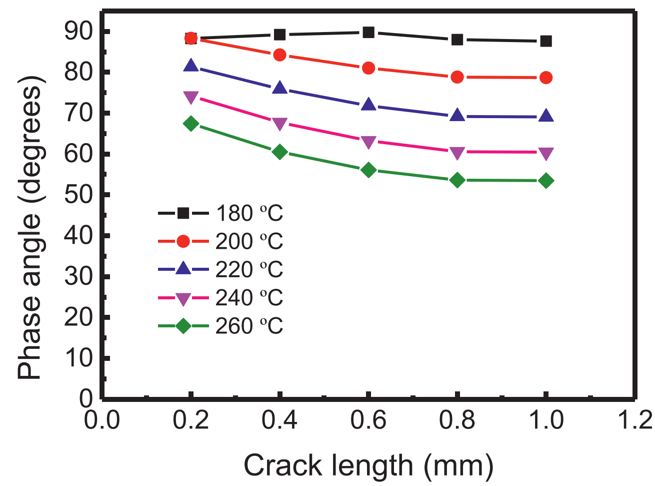

Fig. 19. Phase angle under different crack lengths at bottom die/die attach interface.

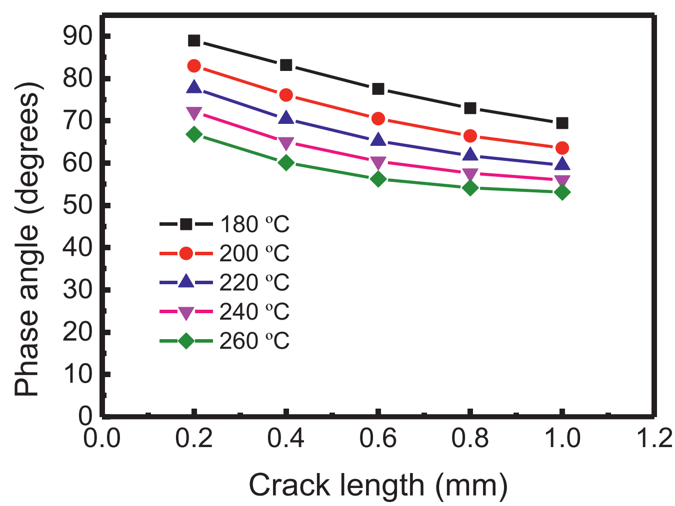

Fig. 20. Phase angle under different crack lengths at bottom die/molding compound interface.

and more significant contribution, which leads to the decrease of mode mixity. The critical interfacial strain energy release rate (or fracture toughness) usually reduces when the mode mixity reduces. The crack has lower phase angle and higher strain energy release rate at 260 °C, therefore the delamination is more likely to happen.

During surface mount reflow, the loading on the moisturized plastic IC package mainly comes from three sources, hygrocopic swelling, thermal expansion and vapor pressure. Figs. 21 and 22 reveal the changes of strain energy release rates over temperature at both bottom die/die attach and bottom die/molding compound interfaces considering the combined effect of three loadings (G_{tot}) as well as the individual effect of hygroscopic swelling (G_h), thermal expansion (G_t), and vapor pressure (G_p). It is discovered that, the strain energy release rates due to hygroscopic loading (G_h) and vapor pressure loading (G_p) are in the similar magnitudes as the strain energy release rate due to thermal loading (G_t). This result implies that, the moisture and vapor pressure play significant contributions to the delamination in the stacked die package in addition to the effect of temperature. Moreover, the relative contribution of the vapor steam and moisture induced swelling is comparable to the effect of CTE mismatch. It can also been seen from that, as the temperature increases, G_t, G_p and G_{tot} show growth while G_h continues to drop. The fact that G_t increases with the growth of temperature is because the reference temperature in this finite

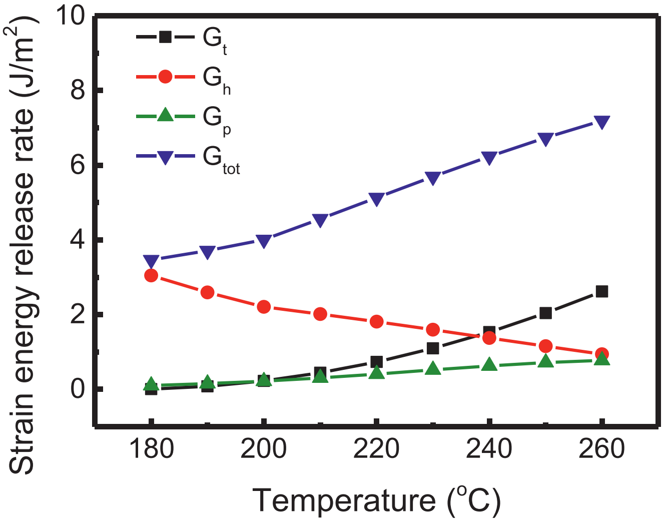

Fig. 21. Variation of G_t, G_h, G_p and G_{tot} with temperature at bottom at bottom die/die attach interface.

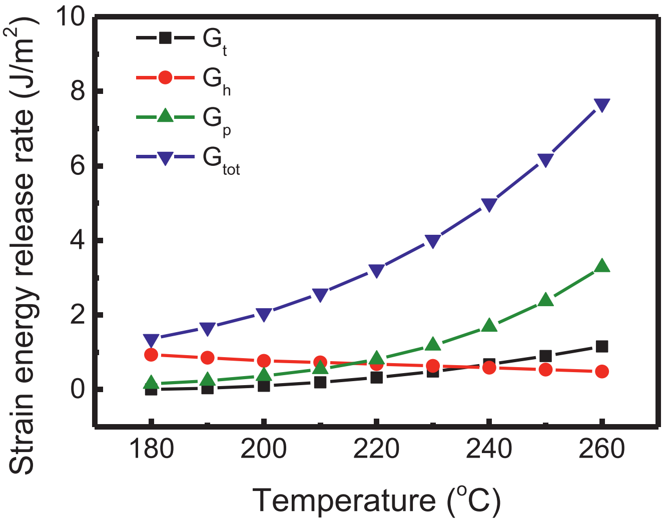

Fig. 22. Variation of G_t, G_h, G_p and G_{tot} with temperature at bottom die/molding compound interface.

element model is set as 175 °C, so the stress due to CTE mismatch will increase as the temperature goes higher than the reference temperature. The vapor pressure related strain energy release rate (G_p) also increases with temperature mainly due to two reasons. Firstly, the vapor pressure induced delamination is more related to the fact that moisture turns into vapor steam. Although the package exterior has significant amount of moisture loss, the package interior especially the die adjacent region still holds lots of moisture. Secondly, the saturated vapor pressure increases exponentially with temperature and the increasing trend is beyond the decreasing trend of moisture content. It should be noticed that, this finite element model only simulates a short time period of reflow process without considering the cooling step. For a real solder reflow process, the moisture desorption happens in a relatively longer time domain, and the moisture content inside the package will continue to decrease. Therefore, both G_h and G_p will continue to reduce until the package is completely dry.

5. Conclusion

This paper provides a comprehensive overview of finite element modeling approaches to study the moisture and vapor pressure induced delamination issue in electronic packaging. Several important topics were covered, including diffusion modeling techniques under dynamic thermal loading, bi-material fracture mechanics modeling methodologies, vapor pressure model and multi-loading boundary conditions. Advantages and disadvantages of different existing moisture related modeling techniques were reviewed and discussed. A novel analogy was proposed for applying the combined hygro-thermal-vapor loading in the finite element modeling, which can reduce users' effort in assigning the multi-loading conditions in the fracture mechanics simulation. Then, a comprehensive and systematic finite element approach was integrated and established to investigate the moisture induced delamination behavior of a stacked die package during solder reflow, including both moisture diffusion analysis and fracture mechanics analysis. The moisture concentration fields at soaking and solder reflow were analyzed. The effect of temperature on the strain energy release rate as well as phase angle was studied. The relationship between initial crack location and the strain energy release rate was also investigated. Moreover, the combined effects of temperature, humidity and vapor pressure on the strain energy release rate evolution during solder reflow were evaluated. The strain energy release rates from integrated loading were compared with that from the individual hygro, thermal and vapor pressure loading conditions. It is shown that the relative contribution of vapor steam and moisture induced swelling is comparable to the effect of thermal expansion mismatch.

CRediT authorship contribution statement

Jing Wang: Conceptualization, Methodology, Software, Writing - original draft. **Yuling Niu:** Conceptualization, Methodology, Validation. **Shuai Shao:** Conceptualization, Methodology, Validation. **Huayan Wang:** Conceptualization, Methodology. **Jiefeng Xu:** Conceptualization, Methodology. **Vanlai Pham:** Conceptualization, Methodology. **Seungbae Park:** Supervision, Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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