Advanced Virtual Testing of Structural Integrity in Microelectronic Assemblies

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Abstract

This work presents some recent progresses in reliability assessment of electronic assemblies in automotive industry and shows how coupled numerical-experimental techniques can help us save time and reduce the cost of IC package qualification. In order to fulfill the continuous trends in miniaturization of the electronic devices together with the demands to shorten the time-to-market, it is essential to use virtual qualification methods with the simulation tools. One of the main concerns in electronic packages is their structural integrity during the fabrication, surface mount process, and service life. A prominent example of failure in electronic assemblies is the interface delamination between two dissimilar materials. This failure mode is accelerated when the polymeric materials absorb moisture from humid environments. Moisture results in degradation of the physical properties of polymers, induces additional deformation due to hygroscopic swelling, and more importantly, degrades the adhesion strength of the polymer to metal joints. This work provides conceptual understandings of the problem of moisture-driven interface delamination in plastic encapsulated microcircuits. In addition, it is shown how the developed method can enhance the material selection in order to improve the delamination resistance in the package and preserve the structural integrity.

1. Introduction

Interface delamination between dissimilar materials is one of the major threats to the structural integrity and reliability of multi-layered structures. In many of these structures, such as microelectronic assemblies, one or more of the materials are made of polymers. In this case, moisture poses a significant threat to the reliability of these products and can be regarded as one of the principal causes of many premature failures [1,2].

Epoxy Molding Compounds (EMCs) are widely used as encapsulating materials in semiconductor packaging industry. The interface between EMC and the copper-based leadframe in plastic IC packages has been found to be one the weakest joints. Most cracks in plastic encapsulated microcircuits initiate and propagate along this interface. The crack propagation facilitates, when the EMC materials absorb moisture from the environment [3,4]. This paper provides a comprehensive overview of the primary mechanisms responsible for the interfacial delamination due to the presence of moisture and shows how coupled numerical-experimental techniques can help us save time and reduce the cost of IC package qualification.

The methodology developed in this study to investigate the interface delamination between epoxy molding compound and the copper-based leadframe of a plastic IC package is as follows:

- Process-induced stresses during the fabrication of the plastic encapsulated devices are taken into account. The method was previously benchmarked by comparing the warpage of a simple biomaterial beam with the results from Finite Element (FE) analysis [2,4].
- Next, the moisture absorption of the plastic package is modeled by FE analysis. In separate studies [1-4] several test specimens were used to investigate the diffusion of moisture in epoxy molding compound and novel simulation techniques were proposed and validated.
- The hygroscopic swelling of the polymers upon moisture absorption is modeled. The value of the coefficient of hygroscopic swelling is determined experimentally and implemented in the FE code [1].
- The adhesion between the epoxy molding compound and leadframe is determined in terms of interfacial fracture toughness. Several test specimens, preconditioning and load setups were used to determine the toughness as function of temperature, moisture and mode angle [4-5].
- Finally, fracture mechanic is applied to analyze the interface reliability. The energy release rate is compared against interfacial fracture toughness and the delamination risk is evaluated.

2. Moisture Diffusion in Plastic Packages

Fig. 1 summarizes a number of effects associated with moisture diffusion in polymeric materials of electronic packages. Obviously, the prerequisite to investigate any moisture effects is to ascertain the diffusion (absorption and desorption) mechanism of moisture. Among the various effects listed in Fig. 1, three mechanisms are extremely important for the reliability of plastic IC packages from the structural mechanics point of view. First, the adhesion between the epoxy molding compound and other package materials (this work focuses on the copper-based leadframe) is of particular importance. This is because of the fact that under poor adhesion, the structural integrity of the package may be threatened, which may lead to disruption in sending electrical signals to the board. Second, the hygroscopic swelling is of particular concern since the resulting dimensional change alters the stress state in these parts. The third mechanism associated with moisture absorption is the effect of vapor pressure. This mechanism has normally significant influence at elevated temperatures of the solder reflow process. The main reason for the vapor pressure effect is the evaporation of condensed water molecules in the molding compound. This is especially important for the lead-free soldering because of the exponential increase of vapor pressure with elevated temperatures. Vapor pressure can be categorized into two types. One type is the micromechanics-based vapor pressure that causes the volume of the molding compound to increase, and hence, causes an additional mismatch between volumetric changes inside the package. The second type is the effect of gathered vapor molecules at delaminated interfaces. This acts as an additional driving force for the crack propagation and finally popcorn cracking of the package.

Presence of moisture in the package is the primary reason for the initiation of interface delamination during the solder reflow process. Moisture diffuses into the package during storage in ambient. The diffusion curve consists of two regions [1]. The first region shows a linear increase in concentration followed by an apparent saturation which can be modeled by a Fickian diffusion model. However prolonged exposure causes an additional linear increase in moisture concentration followed by a secondary saturation region. Therefore the total moisture uptake of the molding compound cannot be modeled using Fick's Law and a more complex model was developed [1] which is applied in this study.

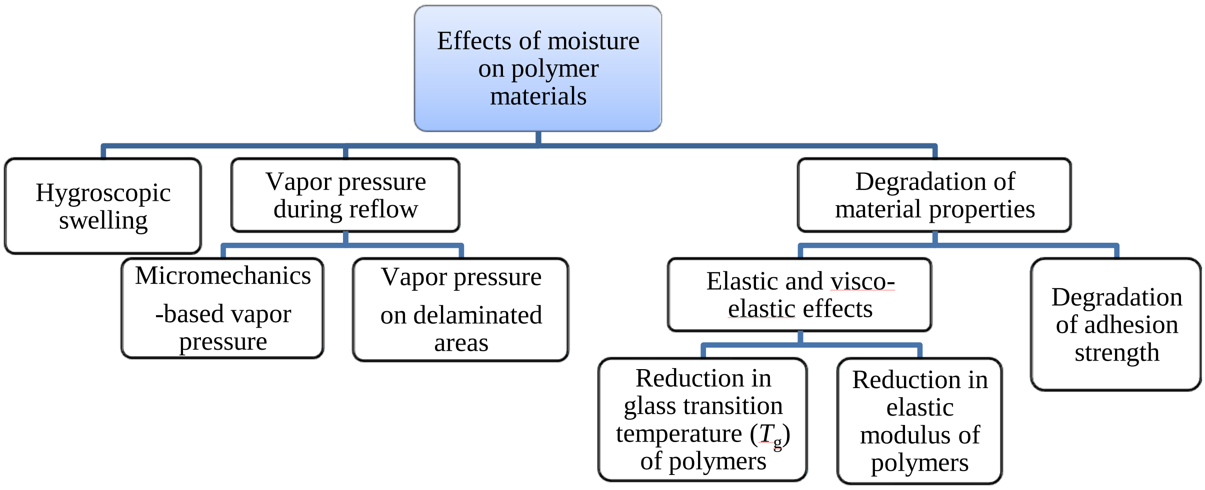


Fig. 1 Effects of moisture on polymeric materials in electronic packages.

3. Moisture Diffusion Tests

A systematic investigation of absorption and desorption of moisture in epoxy molding compounds is explained in Ref. [1]. Absorption of moisture can be explained by an empirical dual-stage non-Fickian behavior. This means that the conventional simulation tools cannot model the diffusion process in epoxy molding compounds correctly and additional consideration is needed for an exact modeling of diffusion behavior. In order to model the moisture diffusion in a plastic IC package correctly, the first step is extracting the non-Fickian material data from the experimental results of standard bulk EMC samples. Fig. 2 shows the recommended methodology to model the dual-stage moisture diffusion in plastic IC packages. The left part of this figure is required to find the non-Fickian diffusion parameters. A simple method to verify these parameters is running the proposed non-Fickian FE analysis by using these parameters and comparing the simulation results with the experimental sorption curves. The next step is implementing these parameters and running an FE analysis for IC packages that share the same molding compound. Obviously, experimental sorption curves of the plastic packages can be used to benchmark the FE results.

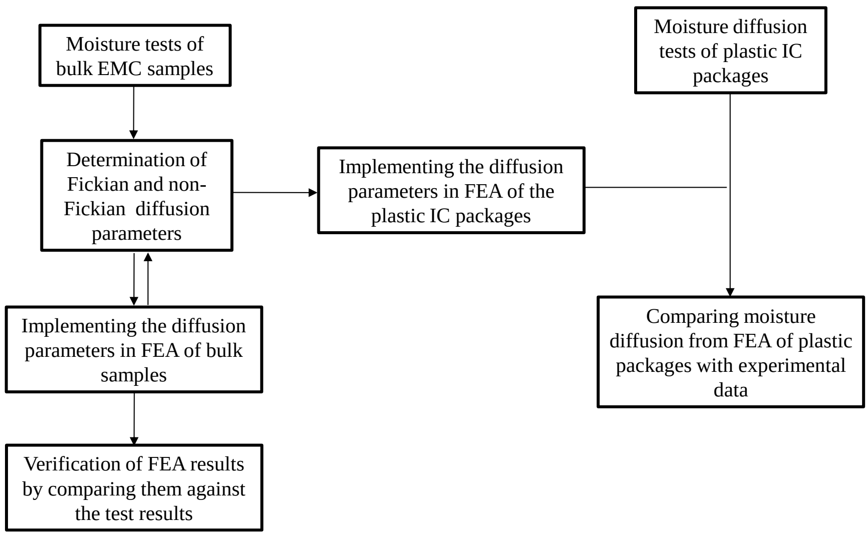


Fig.2 Recommended methodology to investigate the non-Fickian diffusion parameters.

When EMC samples are baked to remove their moisture and to reach a dry state, the sorption history prior to baking was found to play an important role in the desorption curves of these materials. The exposure of an EMC sample upon a virtual saturation (end of the first absorption phase) to a dry environment was found to lead to an almost dry state with only slight residual moisture content at the end. However, a dry state was not achieved when the samples with higher initial moisture content (which were kept in humid environment for a longer time) were baked in dry conditions. A residual moisture content was available upon baking which was a complex function of time, sample geometry and baking temperature. The schematic picture of the influence of sample history may be depicted as shown in Fig. 3.

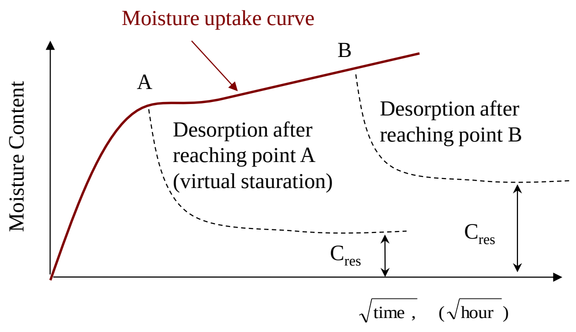


Fig. 3 Schematic model for the residual moisture content upon desorption of moisture.

Samples which reached point A (virtual saturation during the absorption process) show lower residual moisture content upon baking when compared to the samples reached point B (a representative point from the second absorption phase). However, the rate of desorption for both cases was the same, indicating that at least two mechanism are active during the diffusion of moisture. One is a reversible mechanism that dominates the diffusion rate. The other is a non-reversible mechanism that is a function of time, temperature and sample geometry.

The second run of moisture absorption showed also some differences from the first run. The sample sorption history was found to be the dominating factor. The rate of moisture absorption at the second run was found to be higher than that at the first run. The increase in the rate of moisture uptake can be attributed to the formation of new voids in the polymeric materials, which facilitates the transformation of water molecules in the sample. Higher temperatures lead to the formation of more new free volumes. A schematic picture of the effect of sample history on the rate of the second run of moisture absorption may be depicted like the one in Fig. 4.

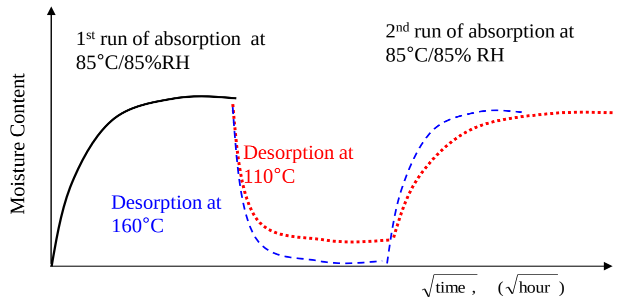


Fig. 4 Schematic model of the second run of the moisture absorption after an absorption/desorption cycle.

4. Fracture Test Results

Electronic packages used in automotive industry are prone to harsh environmental attacks that make the qualification of these devices more challenging than those of packages used in consumer electronics [5-7]. There are typically two environmental effects that influence the structural integrity of these devices. Degradation of the material characteristics during the storage at elevated temperatures and diffusion of moisture prior to surface mount technology and during the service life of these devices pose significant reliability challenges.

By using the Four-point Bending (4PB) delamination tests of EMC/Cu bimaterial samples fracture toughness of this interface under several aging conditions was investigated explained in [1-2]. In the following a summary of fracture results under different testing and aging conditions is presented:

First of all, the test temperature was found to affect the interfacial fracture toughness significantly. It was found that the fracture toughness values demonstrate two scenarios when the temperature rises. First, increasing the temperature from room temperature to the glass transition temperature of the molding compound resulted in an increase in the interfacial fracture toughness. However, the fracture toughness was found to demonstrate an opposite behavior at temperatures above the glass transition temperature of the EMC as shown in Fig. 5. These results can be attributed to two major mechanisms that dominate the adhesion between polymers and metals. The decrease in elastic modulus of EMC with increasing temperature and the increase in the thermal motion of molecules are the primary reasons of adhesion change. In other words, the combination of decrease in Young's modulus and decrease in interfacial interaction at high temperatures determines if the interfacial fracture toughness increases or decreases.

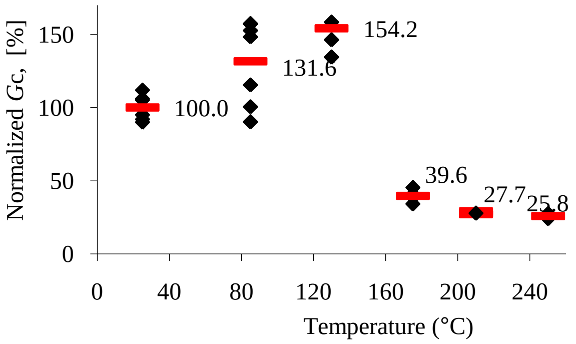


Fig. 5 Effect of test temperature on the interfacial fracture toughness of Cu/EMC interface.

The second problem investigated in this study was the effect of dry aging at elevated temperatures. It was found that the storage of bimaterial samples at temperatures below the glass transition temperature of EMC did not affect the interfacial fracture toughness significantly. However, the storage at 175°C for a period of two weeks caused significant adhesion loss as shown in Fig. 6. There are two mechanisms responsible for this adhesion degradation. The first mechanism was attributed to the degradation of secondary bonds between molecules and atoms of adhesive (here EMC) and substrate (here copper leadframe). The second mechanism impacting the adhesion was found to be the oxidization of the surface of copper leadframe.

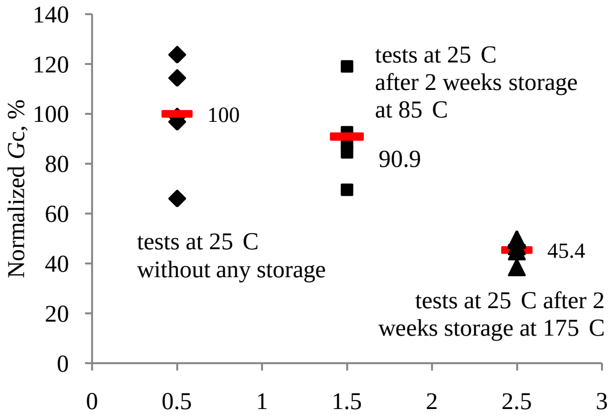


Fig. 6 Effect of 2 weeks thermal storage at 85°C and 175°C dry condition on the interfacial fracture toughness of Cu/EMC.

Finally, the effect of moisture diffusion at 85°C/85%RH condition was investigated in details. Two types of bimaterial samples were used to investigate the effect of moisture on the adhesion between the copper leadframe and EMC layer:

For the samples that allowed for the diffusion of moisture along the interface (Fig. 7), it was found that the rate of adhesion loss was much higher than the rate of moisture diffusion in the bulk EMC layer. This rapid adhesion degradation was attributed to the fact that the diffusion coefficient of moisture at the interfaces is almost an order of magnitude larger than that at a bulk material. This high diffusion rate was attributed to nano- or micro-pores and voids at the interface which facilitate the moisture transfer. Moreover, since these interfaces are under residual stresses, the stresses also contribute to the faster diffusion of moisture.

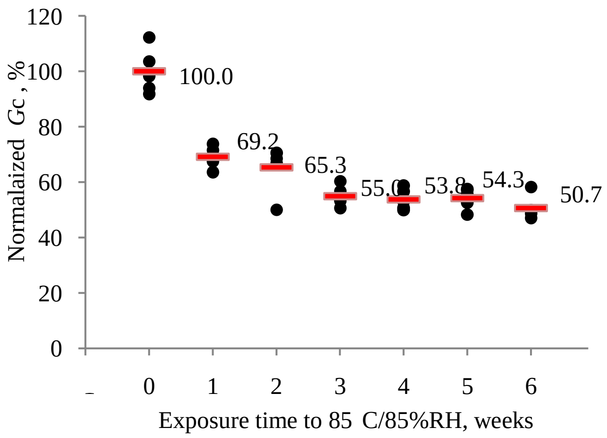


Fig. 7 Effect of interfacial moisture diffusion on the interfacial fracture toughness of Cu/EMC interface.

For the rest of samples the diffusion path from the interface was blocked and diffusion was forced to occur only from the EMC layer (Fig. 8). Consequently, a uniform moisture concentration was available at the interface. Two levels of moisture content (virtual saturation and second phase diffusion) that were identified during the moisture absorption of EMC materials were investigated. Both short term (2 weeks) and long term (4 weeks) sorption conditions resulted in a significant reduction in the interfacial fracture toughness. Similarly to the residual moisture content identified from desorption tests of EMC samples, adhesion recoverability tests were also carried out. For samples that were aged shortly in the humid environment, the adhesion was partially reversible by applying an appropriate heat treatment at 125°C. However, long-term aging in humid condition caused permanent adhesion loss, which was attributed to the degradation of hydrogen bonding between water molecules and polymer chains at the interface.

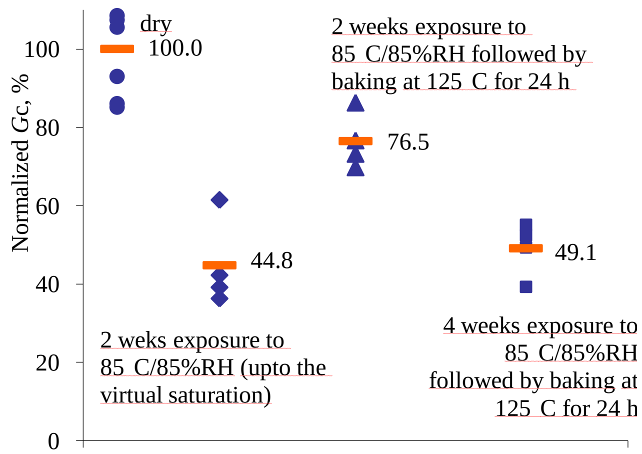
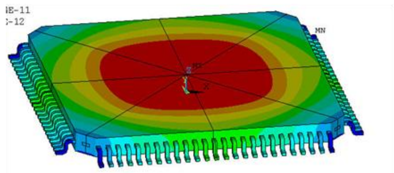


Fig. 8 Effects of moisture absorption, sorption time and the subsequent baking on the adhesion of Cu/EMC interface.

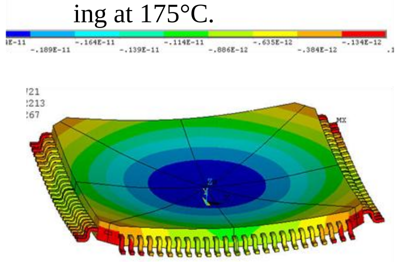
The important result from the moisture diffusion experiments is that the adhesion tests gave reasonable predictive values, in agreement with the observations in moisture absorption and desorption behavior. These realistic test conditions can enable a correlation to the response of microelectronic packages to humid conditions. To the author's best knowledge there is no other evidence in the literature that combines all of the responsible effects for understanding the adhesion degradation mechanism of polymer/metal interfaces. The results of this section provide invaluable information on various effects of moisture-induced adhesion loss, many of which may not direct have to do with moisture, but in reality contribute to the results of fracture tests.

5. Thermo-mechanical Analysis

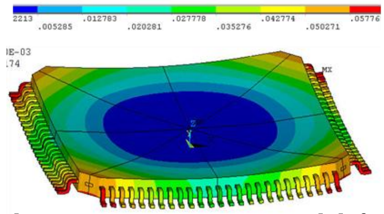
Finite element (FE) analyses were carried out on a TQFP-epad package that uses a commercial epoxy molding compound. This material is completely characterized for a complete thermo-hygro-mechanical FE analysis [1-4]. Fig. 9 shows FE results of this package. Fig. 9a shows the state of the deformations in package during the transfer molding while the epoxy molding compound is still in fluid state. When cross-linking in the EMC material commences, the polymer matrix shrinks and causes deformation of the package at molding temperature as shown in Fig. 9b. When cooling to room temperature, the mismatch between the CTE values of different package materials causes thermal strains to develop. This is the second mechanism causing deformation in the package as shown in Fig. 9c. A third mechanism shown in Fig. 9d is the moisture-induced hygroscopic swelling. Since the chip and leadframe of these packages are impermeable to moisture, the absorption of moisture by EMC materials causes a further deformation in package as shown in Fig. 8d, changing the deformation state from a "smiling" to a "crying" form.



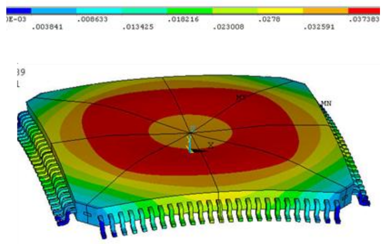
(a) Injection of EMC and transfer molding at 175°C.



(b) Curing at 175°C and deformation due to shrinkage of EMC during the polymerization.



(c) Cooling to room temperature and deforming due to CTE mismatch between package materials.



(d) Further deformation due to the hygroscopic swelling of EMC during moisture absorption.

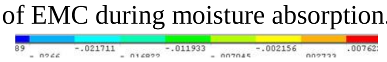


Fig. 9 Deformation of a TQFP-epad package after (a) mold injection (b) manufacturing (c) cooling (d) moisture diffusion.

These examples indicate that any temperature change or moisture absorption can act as a driving force for interface delamination. In the following section the same package will be investigated under temperature cycling test. This example attempts to show how fracture mechanics can be used to predict interface delamination between the copper-based leadframe and epoxy molding compound. By adding a precrack to an interface in the model it is possible to find the strain energy release rate.

6. Fracture Mechanics analysis

In order to estimate the delamination risk based on a fracture mechanics approach, two essential parameters must be estimated and compared to each other. The first parameter is the Strain Energy Release Rate (SERR or shortly *G*) which is the driving force for crack propagation. The second parameter is the critical value of *G*, known as interfacial fracture toughness (G_c) which represents adhesion strength. Ref. [4-8] presents some experimental testing methods, materials characterization techniques, and numerical implementations in order to determine the fracture toughness and viscoelastic behavior of polymers and interfaces.

Once the interfacial fracture toughness is known, it is possible to predict as to whether the loading condition is able to cause an existing crack to propagate. Fig. 10 illustrates the methodology to predict interfacial delamination in plastic IC packages.

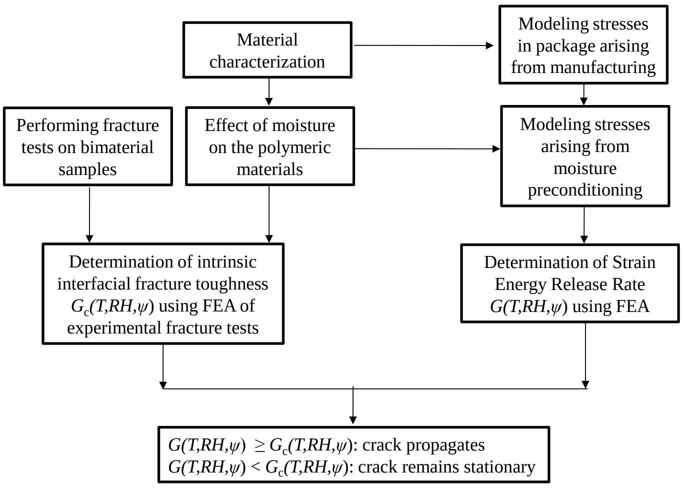
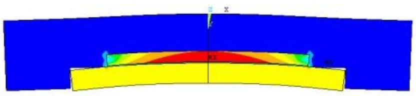
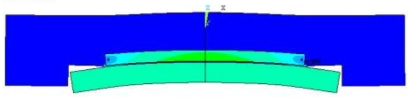


Fig. 10 Methodology to predict the interface delamination by a combined fracture mechanics and thermo-mechanical analysis.

Fig. 11a shows an FE-simulation of the TQFP package with a very short pre-crack length at leadframe/epoxy molding compound interface. The FE model was done using a parametric script for the finite element tool ANSYS. The crack length was varied and the analysis was carried out at each step.



(a)



(b)

Fig. 11 FE modeling the crack at leadframe/EMC interface of a TQFP-epad package. (a) short crack, (b) long crack.

Fig. 11b shows the same package while the pre-crack length was assumed to be quite larger. The nodal loads and displacements were exported for the further post-processing to determine the components of the strain energy release rate. A temperature change of 150°C to -40°C was used as the loading, which mimics the first half of a temperature cycle.

The energy release rate and the mode angle of crack at the leaframe/EMC interface based on the asymptotic linear elastic stress field are determined by Virtual Crack Closure Technique (VCCT). Fig 12 shows the strain energy release rate as a function of the crack length. From this figure it is evident that the energy release rate in this package depends on the crack length at the interface. For short crack lengths the strain energy release rate remains almost constant at moderate values. The *G* value is smaller than the interfacial fracture toughness found in [1-4] for the respective mode mixity. This is in agreement with the experimental temperature cycles performed on these packages, where it was observed that the length of delamination after the solder reflow process determines if the crack would propagate during subsequent temperature cycles. Moreover, as shown in this figure, the mode mixity at the crack tip varies between 4 degrees for very short cracks up to approximately 15 degrees for large cracks of around 1 mm length. This means that the fracture mode in this package is mainly dominated by mode I fracture. Since the interfacial fracture toughness of this interface is known through the experimental part [1-4], it is possible to determine the critical pre-crack length, which leads energy release rate to exceed the interfacial fracture toughness and hence enable crack propagation. Obviously, this critical length of the pre-crack is different for packages that have experiences various humid environments. This is because of the fact that by exposure to moisture the adhesion strength of interfaces decrease as observed in Figs. 7 and 8.

When moisture is available, the first step is to determine the state of moisture concentration. In the most simple form, by assuming one week sorption at 85°C/85%RH the interfacial adhesion is almost 40% lower than that for dry package [1]. Due to the relatively short diffusion path to interface because of thin geometry of package, the moisture concentration may most probably reach the second phase of the absorption curve as described in Fig. 8. This means that there would be no recovery in adhesion when the samples are baked prior to temperature cycle. As a result of adhesion degradation, in the case of one week prior sorption at 85°C/85%RH, the critical crack length of moisture-preconditioned package is almost 0.2 mm. This indicates that crack propagation at the interface of moisture treated samples is possible with smaller initial crack length as compared to dry samples.

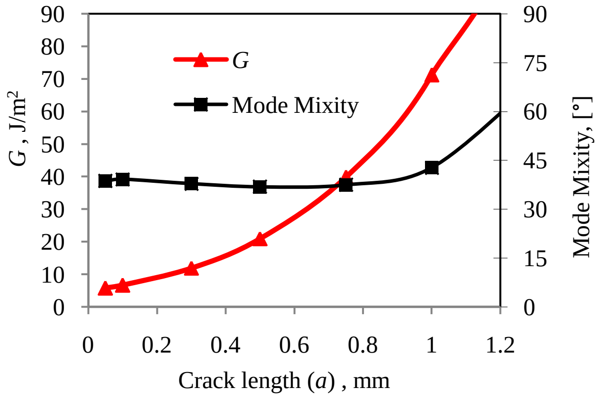


Fig. 12 Strain energy release rate (G) and mode mixity of interfacial crack are plotted as a function of crack length.

7. Conclusions

Due to the complexity of the problems a broad experimental and analytical study was performed to identify the physical mechanisms and the critical factors that influence the loss in interfacial adhesion as a result of moisture. Several micromechanical aspects of the effect of moisture on the epoxy molding compounds were taken into consideration. From a global perspective, the primary aspects considered include moisture diffusion behavior, hygroscopic swelling, and the effect of moisture on interfacial adhesion. Based on the experimental results and on the corresponding numerical analysis, the following fundamental conclusions can be made:

- Moisture transport in epoxy molding compounds shows essentially a non-Fickian diffusion behavior. The moisture uptake curve consists of two parts. The first part is similar to the conventional Fickian curve with a so-called saturation. However, if the samples are exposed to humid environments for a longer period, the second part of the moisture uptake curve, which is a straight line can be observed.
- From the large number of experiments on different sample geometries and preconditioning environments it was concluded that the second linear part of the absorption curve is a nonreversible process and is responsible for a permanent increase in the weight of the plastic parts. In other words, residual moisture content upon desorption tests is the direct consequence of the second linear part of the absorption curve.
- The sorption history of the EMC samples was also investigated. It was observed that, in general, the storage of EMC materials at elevated temperatures results in the formation of new micro-pores in polymers and, consequently, an increase in the diffusivity.
- A remarkable identification from the experimental parts of this study is the difference between the diffusion of moisture through bulk EMC samples and that along the interface between two materials. Two types of experimental analyses support the hypothesis that the diffusion coefficient along the EMC/Cu interface is much larger than that in the bulk EMC sample:
  - First, gravimetric analyses showed that the moisture uptake of structures with interfaces (plastic packages and bimaterial beams) was much faster than that for bulk EMC materials.
  - Second, the adhesion degradation of bimaterial beam samples was found to be remarkably faster than the diffusion of moisture in bulk EMC materials. This suggests that water molecules diffuse much faster along the interfaces and is the reason that the bimaterial samples with unsealed interfaces showed more susceptibility to short-term exposure to moisture than those samples with protected interfacial diffusion path.

In order to use simulation tools for the reliability analysis of plastic IC packages detailed material characterization is required. Several mechanical material parameters were found experimentally. These material parameters are essential for a successful thermo-mechanical FE analysis. However, there are some characteristics that cannot be estimated directly by using the mechanical testing methods. For example, the analysis of stresses by thermo- or hygro-mechanical FE analysis requires the cure shrinkage and hygroscopic swelling coefficient of polymers. These two factors were estimated through a series of experimental-numerical studies as follows:

- The cure shrinkage of the epoxy molding compound due to the polymerization process was found to play a significant role in the overall structural behavior of plastic parts.
- Since the EMC suppliers do not usually provide information on the amount of shrinkage of the materials during the fabrication, a simple bimaterial beam was applied to find the amount of shrinkage. The warpage of the beam was measured at various temperatures, the thermal strains were modeled analytically, and the cure shrinkage was estimated.
- Once the cure and thermal strains and the material constitutive law are known, it is possible to run an FE analysis and find the stresses in the plastic parts.
- Hygroscopic swelling of polymers also contributes to the residual stresses in the multi-layered structures. Depending on the geometry, coefficient of hygroscopic swelling, and the behavior of other materials, diffusion of moisture may increase or decrease the stresses in these samples. It is essential to account for these stresses, because otherwise it may be possible that the state of stress (compressive or tensile) is predicted incorrectly. The simple bimaterial samples were used to estimate the hygroscopic swelling coefficient by warpage analysis.

Adhesion between the epoxy molding compound and the copper-based leadframe was also investigated. It was found that the determination of the intrinsic interfacial fracture toughness requires a detailed understanding of the residual stresses. This means that the analytical solutions for the estimation of the strain energy release rate are not applicable for polymer/metal interfaces because they do not account for the residual stresses. Consequently, in order to determine the intrinsic interfacial fracture toughness of Cu/EMC samples, in this study a series of experimental-numerical analyses were performed as follows:

- First, fracture tests were performed in order to find the critical load that leads to propagation of a precrack at interface. This load was used as an input for the FE analysis of the fracture test.
- Next, the modeling of the fracture test using FE analysis was performed. Since the samples are under residual stresses, the sample fabrication and sorption history was modeled. Then the critical load and the precrack reported from the experimental investigation were modeled.
- Finally a fracture mechanics numerical method was employed and the interfacial fracture toughness was estimated.

A large number of environmental and test conditions were investigated and the effect of each individual factor was studied. The fracture tests results can be summarized in the following statements:

- The effect of test temperature on the interfacial fracture toughness is different for temperatures below and above the glass transition temperature of the EMC materials. While at low temperatures below the glass transition of EMC the interfacial fracture toughness increases with increasing the temperature, the fracture toughness decreases significantly at elevated temperatures above the T_g.
- Aging in dry conditions was also investigated. It was found that the aging at low temperature does not influence the toughness values significantly. However, aging at 175°C caused a remarkable decrease in the interfacial fracture toughness. This can be attributed to the breakage of van der Waals bonds as a consequence of high temperature storage.
- A large number of test specimens were dedicated to the investigation of the effect of moisture on the interfacial fracture toughness. It was found that the presence of water molecules at the interface of the EMC/Cu results in a dramatic loss in the adhesion. However, the storage time in humid environment has a significant effect on the recoverability of adhesion upon baking of the samples.
  - Samples that were stored in humid environment for short time showed higher fracture toughness values after baking in comparison to those samples that were aged for a longer time in humid condition.
  - The main consequence of dual-stage moisture uptake was observed in the fracture toughness results. The effect of second phase of moisture absorption was the destruction of secondary bonds and hence the permanent loss in adhesion strength.

The desorption tests of the bulk EMC samples together with the fracture tests upon baking of preconditioned samples gave a fundamental understanding of the effect of moisture on the EMC materials: The adhesion loss in epoxy molding compounds is due to the replacement of secondary bonds between adhesive and substrate with the hydrogen bonds between water molecules and polymer chains.

The experimental-analytical technique developed in this research could also be extended to account for delamination analysis of plastic IC packages. For example, the delamination risk of a plastic IC package under thermal cycle was investigated. It was shown that the selection of material combination can significantly result in the reduction of delamination risk. This technique could be successfully used to predict the most suitable material and geometry combinations.

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