Cohesive Zone Modeling for Predicting Interfacial Delamination in over mold Components

Sai Krishnan M1, Jeyanthi .S*2, Pradeep Kumar Mani3, Hareesh K T4,M.C Lenin babu5

1,2School of Mechanical and building science, VIT University, Chennai-600127,Tamilnadu,India.
3,4Valeo India Private Limited, CEE DEE YES IT Park, 2nd floor, Block-1, No.63, Rajiv Gandhi Salai, Navalur, Chennai- 600130, Tamilnadu, India. 5Electric Vehicles Incubation and Testing division and School of Mechanical Engineering,VIT Chennai.

Corresponding author’s e-mail address:Jeyanthi.subramanian@vit.ac.in

Abstract. Delamination is one among the significant issues in over molding and electronic packaging. Notably, because of material compatibility and also the weak adhesion-strength of interfaces makes it complex. Typically, delamination takes place at the bimaterial interfaces. In order to predict interface delamination, the cohesive zone technique may be applied as an attainable tool. However, the proper alternative of the cohesive parameters still forms an obstacle for the general usage. The objectives of the work, analytical & numerical modeling of delamination of interfaces between molding compound and metal frames and its subsequent validation using numerical double cantilever beam test and four-point bend tests. In this work, the double cantilever beam and four-point bend tests are used to obtain the strain energy release rate of mode I and mode II values, these values are used as parameters for the cohesive zone method.

1. Introduction

Overmolding is a method in which a single part is producing the usage of or more different materials in combination. Usually the first material, referred to as the substrate, is partially or absolutely covered by next materials (overmold substances) during manufacturing process. Within the overmolding process, the base layer part is molded first, after which the additional plastic layer is molded over and across the original part. The substrate is probably anything like a machined metal component, like threaded inserts, screws, or electrical connectors. In general, interfacial delamination is one of the common failure mechanism in electronic packages, consist of multilayered structures made of dissimilar materials. Interfacial delamination failure includes techniques: crack initiation and crack propagation, numerous experimental setups and theories have been constructed to take a look at these strategies. Amongst that research the cohesive zone approach in various finite element packages are becoming a popular tool for bimaterial interfacial delamination modeling. Cohesive zone modeling for constitute the
delamination behaviour of electronic packaging was reported in various literature. In this work, to identify the interface behaviour of cohesive characterization of copper/PBT GF30 bimaterial, through experiment as well as numerical methods. Parameters that define a cohesive-zone model cannot be measured in conventional away [5], and a well labelled method for acquiring the parameters isn’t available. Special works have prospered in replicating experimental behaviour [6], but a well-designated technique for counting mixed-mode cohesive zone parameters stays lacking. In this work, the resistance of delamination is characterized by fracture toughness (or) strain energy release rate. To measure the delamination fracture toughness, numerical double cantilever beam (DCB) test is used for Mode I (opening mode), and four-point bend test (FPB) is used for Mode II (shearing mode). In this paper, the mode mix dependency was not considered. Energy release rate values obtained from finite element method of double cantilever and four-point flexure tests are given to the parameters for cohesive zone method which will be explained in the below 3.1 and 3.3 sections.

2. Experiment setup

Test sample consists of the copper lead frame over mold with the PBT GF30 which is thermoplastic material. PBT means polybutylene terephthalate which is grouped under the thermoplastic material family, 30% of glass fiber added that is why it’s represented as the PBT GF30, because of extra added glass fiber, the material behaves excellent mechanical strength and great dimensional accuracy in a wide temperature range. Copper lead frame consists of total length 70 mm, and width of copper is 9mm and total plastic overmold a length of 55 mm, and also width of plastic material 11mm.

The sample is tested in the tensile test machine as shown in figure 1. The sample is vertically placed in the two dies. For bottom die, sufficient pressure is applied for holding purpose, feed rate is given as 2mm/min, load vs displacement data as recorded and shown in figure 2

2.1. Load Vs displacement
From the load vs displacement data, for the sample 1 peak load or critical load observed is 1272.61N. At this critical load separation has started between metal and plastic. For the sample 2 critical load observed at 1306N. From the load displacement data, for the sample 1 and sample 2 delamination separation starts at the average of 1.27kN to 1.3kN. Up to the 1.3kN interface bonding behaves like a linearity, the point at which it loses its stiffness the curve follows the nonlinear behaviour. The following figure 3 shows after and before the test samples.

Figure 3 Sample after and before experiment

3. Energy release rate via VCCT

In this work, numerical and analytical bimaterial double-cantilever beam (DCB) and four-point bend (FPB) test have been performed to determine the strain energy release rate for near opening and shear loading conditions for PBTGF30&copper bimaterial interface, by using the virtual crack closure technique (VCCT). Obtained energy release rate values are assigned as parameters for cohesive layer in between metal and plastic interface and then simulating load displacement data with cohesive-zone finite element modeling.

\[
G = -\frac{d\Pi}{dA} \tag{1}
\]

Where \(G\) is the energy release rate which is calculated from finite element method over the virtual crack closure technique (VCCT) first presented by rybicki and kanninen [9], and in a while enhanced for 3D-cases by krueger [10]. They showed a way for calculating the strain energy release rate in the finite element method. In this work mode mix dependency was not yet considered. VCCT calculates energy-release rate, with the assumption that the energy required to separate a surface is the same as the energy required to close the same surface [10], and also assumes that stress states near the crack tip do not change significantly when the crack grows by a small amount. For 2-D crack geometry with a low-order element mesh, the interfacial toughness is defined as

\[
G_I = -\frac{1}{2\Delta a} R_y \Delta \nu \tag{2}
\]

\[
G_{II} = -\frac{1}{2\Delta a} R_x \Delta u \tag{3}
\]

Where \(G_I\) and \(G_{II}\) are mode I and II energy-release rate, respectively. \(\Delta u\) and \(\Delta \nu\) are relative displacement between the top and bottom nodes of the crack face in local coordinates x and y,
respectively, and $R_x$ and $R_y$ are reaction forces at the crack-tip node. $\Delta a$ is crack extension, as shown in the following figure 4.

![Figure 4 2D crack geometry schematic](image)

### 3.1. Finite element procedure of double cantilever beam test

The test is used to calculate the initiation and propagation value of opening mode under cyclic as well as static loading situations. The dimensions of finite element model consist, length of 100 mm was considered for both copper and PBT GF30 material. Thickness of copper considered as the 1.5 mm and thickness of PBT GF30 considered as 2.6 mm. Width of 9 mm considered for both copper and PBT GF30, a predefined varying crack was assigned in between copper & PBT GF30 interface. Finite element model of DCB was shown in figure 5.

![Figure 5 loading and boundary condition of copper and PBT GF30 double cantilever beam specimen](image)

Material properties of copper and PBT GF30 are mentioned below table 1

| Sl. No. | Material     | Young's modules (E) | Poisson's ratio (μ) |
|---------|--------------|---------------------|---------------------|
| 1       | Copper       | 121 GPa             | 0.33                |
| 2       | PBT GF30     | 9.7 GPa             | 0.35                |

Proper boundary conditions and loading are essential for any finite element simulation. In this analysis at the right end of the cantilever beam all degrees of freedom constrained, and at the left end of the beam the average value of critical load i.e $P_{cr} = 1.29$ kN is assigned, for bottom portion of left end of beam all degrees of freedom is constrained. In this simulation we used ANSYS® apdl 18.2 version. For both copper and PBT GF30, structural solid element was used. Some assumptions taking into considered for analysis they are: For PBT GF30 material linear elastic property was considered because at room temperature PBT GF30 behave like elastic material and also delamination process considered to be quasi static process. The numerical simulation is performed for various crack lengths for $1 \text{ mm} \leq a \leq 6 \text{ mm}$. The important consideration about the finite element analysis of DCB test, strain energy of mode I value is varied until the simulated load vs displacement graph closely.
matches the experimental data \[17\]. Average value of strain energy up to crack length of 6 mm obtained by finite element method 7.56 N/mm.

3.2. Double cantilever beam analytical calculation

For a bimaterial interface with layers of distinct materials, a robust analytical answer for strain energy release rate isn't available. Some sources provide derivations from plate theory or stress intensity factor analysis that results in complicated equations \[12\], the compliance technique can be applied by using treating the thinner layer as a single cantilever beam \[14\]. A modified compliance technique may produce a great approximation for cracks with various thickness \[13\]. On this technique, the layers of the DCB specimen are treated as separate cantilever beams, resulting within the following equation from soboyejo et al. for mode I SERR \[11\].

\[
G = \frac{6P}{E_{PBT}b^2t_{PBT}} \left(1 + \frac{1}{\beta_T^2}\right) \\
\beta_T = \frac{E_{Cu}}{E_{PBT}} \\
\beta_E = \frac{E_{Cu}}{E_{PBT}}
\]

Where \(G\) is the strain energy release rate for opening mode loading, produced by the DCB loading configuration from applied load \(P\) and also \(a\) is the crack length and \(b\) is specimen width. \(\beta_E\) is the stiffness ratio between copper and PBT GF30, and \(\beta_T\) is the thickness ratio. Material property young’s modules appears in Table.1 for both materials. Knowledge of crack length \(a\) is required to apply this formula, all obtained analytical strain energy release rates values are summarized and average value of strain energy up to 6mm delamination length obtained by analytical method = 7.68 N/mm, which is much less than 3% distinct from the average value computed using VCCT.

3.3. Four point bend test numerical modeling

The four-point bend (FPB) test is one of the popular test to find out strain energy release rate characterization because it gives strong delamination in the interface and does no longer rely on length of the crack. To calculate the strain energy release rate with the FPB test, the VCCT technique was applied using finite element method by using ANSYS®, a 3D model of the FPB test is prepared. For both copper and PBT 30GF 8-node structural solid element was assigned. The dimensions of finite element model consist of the, width of the copper and PBT GF30 considered as the 9mm and thickness of copper and PBT GF30 considered as the 1.5 mm and 2.6 mm respectively. The total length of the model is 100 mm. The crack length is 9 mm on both side of the symmetry line.

![Finite element result of the four-point bend specimen with interfacial crack](image)

The distance between inner supports is 74 mm, and the outer rollers separated by 90 mm with force \(P_{out}\). To decrease the computation time, a one-half symmetry model is considered for simulation. Both copper and PBT 30GF are assumed to be linear elastic at room temperature. Material properties are assigned for this analysis are from Table 1. Nodes of copper at the boundary of symmetry have displacement was constrained in the direction of x. At the narrow support pin, y- directional displacement that is vertical displacement is constrained, the contours of near crack stress field are shown in figure 6.
Initial simulations do not show crack-interpenetrations and stresses are primarily tensile, so contact pairings are not used in the model. The FPB model shows similar stress contours to those at the DCB crack tip. The contours are asymmetric due to the dissimilar layers. The stresses vary with distance and angle from the crack tip. The maximum von mises stress is found to be below the copper yield stress, so the elastic assumption is accepted. Average value of mode II strain energy release rate value obtained from finite element analysis was $G_{II} = 12.96 \text{ N/mm}$.

### 3.4. Four point bend test analytical calculation

For the bimaterial interface, strain energy release rate can be calculated by the following equations from Charalambides et al. [15]. $I_C$ is the area moment of inertia of the copper, while $I_C$ is the area moment of inertia of the overall composite beam. $\lambda$ is a non-dimensional parameter that gives the stiffness ratio between copper and PBT GF30, FPB test was independent of arbitrary crack length [15], so for this study a crack length of 9mm as considered. Average strain energy release rate is obtained by calculating $G_{II}$ during the steady-state delamination, $G_{II} = 13.1 \text{ N/mm}$. In this work analytical and finite element method calculations of $G_{II}$ for the FPB test assume a perfect symmetry within the specimen.

\[
G_{II} = \frac{(1-\mu_C^2)EI^2}{8b^2I_C} \left( \frac{1}{I_C} - \frac{\lambda}{I_C} \right) 
\]

\[
I_C = \frac{t_C^3}{12} 
\]

\[
\lambda = \frac{1-\mu_{\text{PBT}}}{1-\mu_C} 
\]

\[
I_C = \lambda I_C + \frac{t_{\text{PBT}}^3}{12} + \frac{\lambda I_C t_{\text{PBT}}(I_C + t_{\text{PBT}})^2}{4(\lambda I_C + t_{\text{PBT}})} 
\]

### 4. Interface cohesive zone modelling

Interface delamination failure include techniques of crack initiation and crack propagation. Numerous experimental setup and theories have been constructed over the years. Amongst that research the cohesive zone approach as being carried out in various finite element packages is becoming a popular tool and also, for cohesive zone method does no longer require starter cracks. Accordingly, Cohesive zone modeling is perfectly suitable for interfacial cracking since such cracks generally tend to propagate alongside the interfaces of a structure. Parameters that describe a cohesive zone model cannot be determine straight away [5], and a well designated method for getting the parameters isn’t available yet. So far special works have succeeded in repeating experimental behaviour [6], but a well-described technique for enumerating mixed-mode cohesive zone parameters stays lacking. In this finite element cohesive method, strain energy release rate values gained from the numerical double cantilever beam test and four-point bend test are used has the parameters for the interfacial cohesive elements. In a cohesive zone model, cohesive elements are placed along material interfaces. Science the model is symmetric about the x-axis. In this study one half the model is considered for the simulation, thickness of copper considered as the 0.75 mm and thickness of PBT GF30 taken as the 1.3 mm and length of copper considered as the 70 mm and length of PBT GF30 considered as the 55 mm replicating the original specimen model. The bottom portion of PBT GF30 nodes is constrained in all degrees of freedom, and nodes of copper elements are constrained in all degrees of freedom except in translation y, and also enforced displacement of 2mm/min given to the translation of positive y-direction. The cohesive finite element model shown in the figure 7.
For both copper and PBT GF30 finite element models, 8-noded structural solid element was assigned. For mesh, aspect ratio 1 is maintained throughout the mesh geometry. Cohesive elements i.e. inter205 elements are placed in between copper and PBT GF30 interface. From finite element model the load-displacement data releases the critical forces and displacements for delamination as well as initial loading stiffness behaviour.

4.1. Correction factor

In actual sample there is total of 1135 mm² mating surface area between metal and plastic but in simulation 86% area only considered due element capability.

For this reason, we are getting a more deviation. For the actual consideration of total surface area, due to the linearity, width of the FEA model increased from 9mm to 10.5 mm to compensate the total surface area and then performed the same above-mentioned finite element analysis. After the correction factor has done, finite element analysis performed as mentioned above procedure and load displacement data has recorded, this time critical load observed at the 1158.3N which is less than the 10% deviation.

4.2. Experiment Vs Numerical results

From the experiment, average critical load identified from the range of 1.25kN to the 1.3kN. From the simulation, load displacement data critical load observed less than 10% deviation from the experiment which is 1158.3N.
4.3. Challenges involved in cohesive zone modeling
When cohesive zone method is used with finite element analysis, delamination path must be known priori in order to place the cohesive elements appropriately in a finite element mesh and also cohesive zone elements capable of creating in flat surfaces only. The cohesive zone method strategies are difficult for predicting crack growth inside a solid body under general loading conditions. The cohesive zone method strategies best suited for monotonic loading conditions.

5. Conclusion
An attempt was made for understanding the interface behaviour of copper/PBT GF30 materials. From this work we identified the copper/PBT GF30 cohesive characteristic behaviour, which follows the exponential cohesive behaviour. Based on experimental data, critical failure load identified for the Copper/PBT GF30 interface. Parameters required for cohesive zone method were identified, to do so numerical double cantilever beam and four-point bend test were performed. While performing the DCB and FPB test, critical load as considered from the experiment data. Based on fracture mechanics technique requires the calculation of fracture parameters, which can be extracted from finite element analysis results using the virtual crack closure technique. This study is useful for the better understanding of the interface behaviour of copper/PBT GF30 interface for future models.

References
[1] Naghipour P, Bartsch M, Voggenreiter H. Simulation and experimental validation of mixed mode delamination in multidirectional CF/PEEK laminates under fatigue loading. International journal of solids and structures. 2011 Mar 15;48(6):1070-81.
[2] Biel A, Alfredsson KS, Carlberger T. Adhesive tapes; cohesive laws for a soft layer. Procedia materials science. 2014 Jan 1;3:1389-93.
[3] Zhang B, Yang D, Ernst L. Cohesive zone modeling of mixed-mode delamination test. In2013 14th International Conference on Electronic Packaging Technology 2013 Aug 11 (pp. 559-565). IEEE.
[4] Zhang W, Yang D, Ernst L, Zhang B, Yang W, Cai M. Interface crack propagation between epoxy moulding compound and copper. In2016 17th International Conference on Thermal, Mechanical and Multi-Physics Simulation and Experiments in Microelectronics and Microsystems (EuroSimE) 2016 Apr 18 (pp. 1-8). IEEE.
[5] Mei H, Gowrishankar S, Liechti KM, Huang R. Initiation and propagation of interfacial delamination in integrated thin-film structures. In2010 12th IEEE Intersociety Conference on Thermal and Thermomechanical Phenomena in Electronic Systems 2010 Jun 2 (pp. 1-8). IEEE.
[6] Raghavan S, Schmadlak I, Leal G, Sitaraman SK. Framework to extract cohesive zone parameters using double cantilever beam and four-point bend fracture tests. In2014 15th International Conference on Thermal, Mechanical and Multiphysics Simulation and Experiments in Microelectronics and Microsystems (EuroSimE) 2014 Apr 7 (pp. 1-5). IEEE.
[7] Liu S, Mei Y, Wu TY. Bimaterial interfacial crack growth as a function of mode-mixity. IEEE Transactions on Components, Packaging, and Manufacturing Technology: Part A. 1995 Sep;18(3):618-26.
[8] Tran HT, Shirangi MH, Pang X, Volinsky AA. Temperature, moisture and mode-mixity effects
on copper leadframe/EMC interfacial fracture toughness. International Journal of Fracture. 2014 Jan;185(1):115-27.

[9] Rybicki EF, Kanninen MF. A finite element calculation of stress intensity factors by a modified crack closure integral. Engineering fracture mechanics. 1977 Jan 1;9(4):931-8.

[10] Krueger R. Virtual crack closure technique: history, approach, and applications. Appl. Mech. Rev. 2004 Mar 1;57(2):109-43.

[11] Soboyejo WO, Lu GY, Chengalva S, Zhang J, Kenner V. A modified mixed-mode bending specimen for the interfacial fracture testing of dissimilar materials. Fatigue & Fracture of Engineering Materials & Structures. 1999 Sep;22(9):799-810.

[12] Sundararaman V, Davidson BD. An unsymmetric double cantilever beam test for interfacial fracture toughness determination. International journal of solids and structures. 1997 Mar 1;34(7):799-817.

[13] Xiao F, Hui CY, Kramer EJ. Analysis of a mixed mode fracture specimen: the asymmetric double cantilever beam. Journal of Materials Science. 1993 Oct;28(20):5620-9.

[14] Cao HC, Evans AG. An experimental study of the fracture resistance of bimaterial interfaces. Mechanics of materials. 1989 Jun 1;7(4):295-304.

[15] Charalambides PG, Lund J, Evans AG, McMeeking RM. A test specimen for determining the fracture resistance of bimaterial interfaces.

[16] Auersperg J, Dudek R, Michel B. VCCT and integral concepts of bi-material interface fracture in low-k structures—Going to understand relation. In2010 12th Electronics Packaging Technology Conference 2010 Dec 8 (pp. 632-636). IEEE.

[17] Kwatra A, Samet D, Sitaraman SK. Effect of thermal aging on cohesive zone models to study copper leadframe/mold compound interfacial delamination. In2015 IEEE 65th Electronic Components and Technology Conference (ECTC) 2015 May 26 (pp. 1531-1537). IEEE.

[18] Shirangi MH, Wunderle B, Wittler O, Walter H, Michel B. Modeling cure shrinkage and viscoelasticity to enhance the numerical methods for predicting delamination in semiconductor packages. InEuroSimE 2009-10th International Conference on Thermal, Mechanical and Multi-Physics Simulation and Experiments in Microelectronics and Microsystems 2009 Apr 26 (pp. 1-8). IEEE.