Core Crack Mitigation in Semiconductor Substrates: A Multi-Scale Simulation Approach to Design Organic Core Material Properties

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Abstract

In advanced semiconductor package**,** organic core materials are widely used. It is essential for ensuring mechanical reliability, yet cracks can occur within the organic core under thermal loading. However, guidelines for designing core materials that suppress these cracks without increasing warpage of the semiconductor package have not yet been established. Here, we present a two-step multi-scale simulation approach to optimize the organic core material properties used in advanced semiconductor packages, focusing on mitigating core crack initiation without increasing package warpage. In the first step, the effective anisotropic properties of a composite core material —consisting of resin and glass cloth—are computed through homogenization methods to establish a macro-scale model of the flip chip ball grid array structure. In the second step, localized finite element simulations utilizing representative volume elements are performed to investigate the stress distribution in the microstructure, particularly at free edge regions prone to cracking. The simulation results demonstrate that controlling the resin's through-thickness (out-of-plane) coefficient of thermal expansion (CTE) can reduce local tensile stresses responsible for crack initiation without notable increases in board warpage. In addition, thermal-shock experiments confirmed the same trends obtained from the simulations and provided practical validation of our design guidelines. In summary, this integrated approach offers a practical route to engineer core materials that both prevent cracking and limit warpage in semiconductor packages.

Key words

Semiconductor Package, Organic Core Material, Multi-Scale Finite Element method (FEM), Coefficient of thermal expansion (CTE), Thermal Stress Analysis

I. Introduction

Recent advances in artificial intelligence, such as large language models, and the development of next-generation communication systems like 6G have created a strong need for fast data transfer and wide bandwidth. These requirements push the semiconductor industry to improve their performance. As a result, semiconductor packages have been becoming larger and more complex [1]–[6]. Notably, advanced packaging techniques now often rely on heterogeneous integration, in which individually fabricated components are assembled together. This approach has led to the development of sophisticated packaging structures, including 2.1D, 2.3D, and 2.5D configurations that commonly utilize interposers for integration [3]–[6]. Because these packages are growing in size and complexity, the substrate materials that support them must meet more stringent mechanical reliability requirements. For example, they must keep low warpage, board level reliability and crack-free [7], [8].

Warpage in semiconductor packages is largely caused by the mismatch in coefficients of thermal expansion (CTE) between silicon-based components (such as chips and interposers) and substrate material.

To reduce the warpage, it is essential to design substrate materials whose overall CTE values closely match that of silicon; in general, materials with lower CTE and higher elastic modulus are more effective in suppressing warpage [9], [10].

Substrates are typically composed of a core layer and build-up layers. Substrate materials typically employ an organic core material comprised of glass cloth and organic materials. In this case, an organic core is created by laminating prepregs made by impregnating glass cloth with a mixture of resin and fillers. Build-up layers are formed by laminating insulation films and forming wiring on both the top and bottom of the core. Through forming the solder resist and bumps (or bump soldering), the substrates are completed.

It is clear that using low-CTE core materials can significantly reduce warpage. Resonac Corporation (the authors' affiliation) has provided various substrate core materials, including MCL-E-705G, MCL-E-795G, and MCL-E-795G (LH type), in response to the increasing demand for lower warpage. For instance, MCL-E795G (LH type) exhibits a CTE in the range of 4.5–6.5 ppm/K (TMA method compression mode). Furthermore, low-CTE glass core materials have also been developed. However, on the other hand, this approach may introduce a CTE mismatch between the core material and the build-up layers. Such a mismatch can create high local stresses that lead to crack initiation and propagation, especially prominent along free edges of core material, whether the core is organic or glass [11]–[13]. Balancing the CTE of the core with that of the build-up layers may mitigate these stresses but might compromise the advantage in controlling warpage. Finding an effective solution for both issues remain challenging [12].

In tackling these challenges, due to the complexity of advanced semiconductor packages, experimental studies alone are often not enough. This is because physical testing can be limited by fabrication challenges, high prototyping costs, and difficulties in capturing local stress concentrations. Instead, numerical and theoretical methods are widely used to evaluate package reliabilities [14]–[17].

For simpler, symmetrical structures, basic theoretical models have been developed to explore general relationships between materials and warpage behavior [15]. These models provide a foundational understanding for warpage or stress distributions. For more complex designs, finite element method (FEM) simulations have been widely used to analyze the detailed stress distributions within the package [14]–[17]. These simulations allow for a deeper and more precise evaluation of local stresses, even in cases where experiments are challenging.

In this study, we use a two-step multi-scale FEM analysis to tackle these challenges (shown in Fig. 1). In the first step,

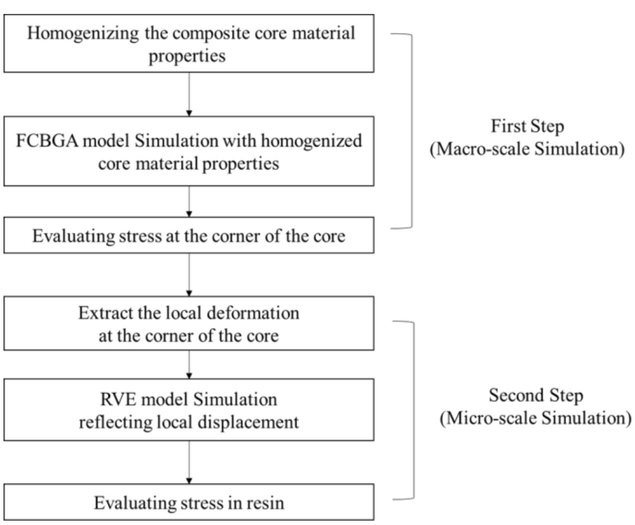

Fig. 1 Two-step multi-scale simulation procedure

we determine the effective anisotropic properties of the composite core by homogenizing the resin and glass cloth materials. This allows us to model the FCBGA structure at the macro level, including core properties that reflect the respective material characteristics of resin and glass cloth. In the second step, we analyze representative volume elements (RVEs) to examine the stress distribution at the micro level reflecting the core-corner strain obtained from the macro model. Our results show that lowering the resin's out-of-plane CTE—while keeping its in-plane CTE unchanged—can reduce the local tensile stresses that lead to cracks, without increasing package warpage and other stresses.

These findings improve our understanding of stress behavior in organic core materials and provide practical design guidelines to enhance the mechanical reliability of advanced semiconductor packages.

II. Method

A. Simulation Method

The issue of core cracking in advanced semiconductor packages primarily results from localized stress concentrations at the free edges of the substrate during thermal loadings, such as thermal cycle and thermal shock. To evaluate these stresses, a comprehensive two-step multi-scale FEM simulation approach was implemented using ANSYS Mechanical 2023R2 (ANSYS Inc.). This approach combines macro-scale thermal–structural analysis of a simplified flip-chip ball grid array (FCBGA) structure with micro-scale analysis focused on detailed stress distributions within the composite core material.

The first step in the simulation workflow addressed the overall thermal–structural behavior of the FCBGA package, focusing on the cooling phase of a thermal cycle — a critical condition for stress accumulation and crack initiation. The FCBGA configuration consisted of a die size of 50 mm × 50 mm and a substrate size of 120 mm × 120 mm with an 8-2-8 arrangement of build-up layers (shown in Fig. 2). The core thickness was 800 μm. Other information of the structural components, including thickness, CTE and elastic modulus, are listed in Table I. To accurately describe the composite core material geometry and its anisotropic mechanical properties, homogenized CTE and elastic modulus values were derived using the MaterialDesigner tool in ANSYS Mechanical. These values represented the combined behavior of the resin and glass cloth constituents in the core material. To calculate homogenized properties, RVEs model was prepared. The RVE model incorporated both resin and glass cloth constituents, shown in Fig. 3. The geometry of the RVE was defined as a block with dimensions of 92 μm thickness and 141 μm in-plane length. The properties of the core's representative constituent materials are listed in Table II. These include key parameters such as CTE and elastic modulus for both the resin and glass cloth. By combining these materials in the RVE model, we calculated the anisotropic material properties of the composite core material. The results of this computation are summarized in Table III. These calculations provide a detailed representation of the composite material's anisotropic mechanical properties.

The material properties obtained from this analysis were then employed in the macro-scale FCBGA model during the first step of the simulation. This ensured that the simulation of the thermal–structural behavior reflected the actual mechanical characteristics of the composite core material.

The simulation utilized a quarter-symmetric model of the FCBGA package to reduce computational costs while allowing detailed evaluation of warpage and thermal stresses. Non-linear thermal–structural analysis was conducted to account for large deformations. The mesh consisted of six-node hexahedral second-order elements, and the total element count for the macro-scale model was 252,724. A stress-free reference state was defined at 190 °C, and the displacement and stress were evaluated at –55 °C to simulate typical cooling conditions during a thermal cycle. The results of this step provided key insights into package warpage and stress distributions at critical locations in the package. Warpage was evaluated by measuring the vertical difference between the center and the edge of the FCBGA package bottom surface. Crack initiation typically occurs at the free edge of the core. However, the vertical position of crack initiation depends on the core material and construction. In the present simulation, high stress was observed in the central region along the height, rather than at the upper or lower ends, which is consistent with the findings reported in [12]. Therefore, the stress evaluation in this study focused on the core mid-height.

The second step employed micro-scale analysis using a RVE model to investigate localized stress distributions within the composite core material. Boundary conditions derived from the macro-scale simulation were applied to the RVE to capture the detailed stress behavior at the free edges of the core. These boundary conditions represented the strain state induced by the macro thermal–structural deformation of the FCBGA package. The RVE model consisted of a 2×2×3 configuration (shown in Fig. 3), allowing detailed analysis of stress concentrations within the composite material.

The mesh of RVE model for this step was constructed using four-node tetrahedral second-order elements to accurately handle the complex geometry of the composite material, resulting in a total element count of 1,176,050 for the RVE. The analysis focused on evaluating out-of-plane tensile stresses at the mid-thickness of the core, as these stresses are most strongly correlated with resin cracking.

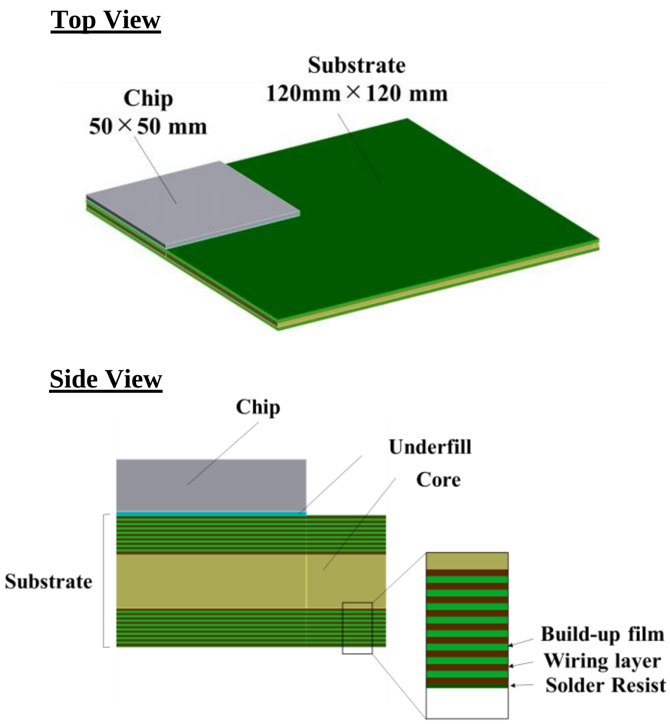

Fig. 2 Simulation model for FCBGA structure

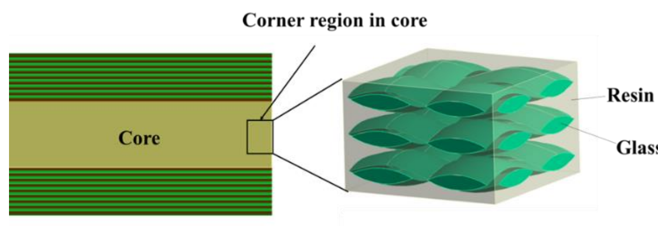

Fig. 3 RVE model of core structure

Table I. Material properties of FCBGA Structure at 25 °C

Material	Thickness [μm]	CTE [ppm/K]	Elastic Modulus [GPa]
Chip	775.0	3.2	167.0
Underfill	60.0	20.0	11.0
Solder Resist	18.0	30.0	4.0
Wiring layer	35.0	20.3	39.1
Build-up film	30.0	34.0	5.5

Table II. Material properties of core Material

Material	CTE [ppm/K]	Elastic Modulus [GPa]
Resin	30.0	5.0
Glass	5.0	73.0

Table III. Example of calculated core material properties

Direction	CTE [ppm/K]	Elastic Modulus [GPa]
X-direction (in-plane)	8.9	23.6
Z-direction (out-of-plane)	20.8	10.1

In practice, glass cloth is inherently distributed non-uniformly, and cracks may initiate within the resin matrix, at the resin–glass-cloth interface, or inside the glass cloth itself. This study specifically focused on stress evaluation in resin-rich regions. The evaluation point was set at the height center position of the resin free edge. The free edge of the core was left unconstrained in the simulation to replicate realistic stress environments during thermal cycling.

To gain a deeper understanding of the stress mechanisms in the core material, four simulation cases were conducted:

Glass cloth variation: A variety of glass cloth is commercially available, and it is well established that employing low-CTE, high-modulus cloth can reduce the composite-core CTE and thereby mitigate package warpage. In this study, two representative reinforcements were examined: Glass A, a high-CTE, low-modulus grade, and Glass B, a comparatively low-CTE, high-modulus grade, shown in Table IV.

Table IV. Material properties of glass cloths

Material	CTE [ppm/K]	Elastic Modulus [GPa]
Glass A	5.0	73.0
Glass B	2.6	85.0

Isotropic Resin: The resin in the composite core was modeled with an isotropic CTE, which was varied among 30, 45, and 60 ppm/K. This case evaluated the relationship between resin CTE and core stress at corner.

Anisotropic Resin: The resin was modeled with independent in-plane and out-of-plane CTE values to account for potential anisotropy induced by material composition. In-plane CTE was fixed at 30 ppm/K, while out-of-plane CTE was varied to achieve anisotropy, which is quantified by calculating the ratio of the out-of-plane coefficient of CTE to the in-plane CTE of the resin, ranging from 1.0 to 2.0. This case aimed to explore how anisotropic resin properties influence localized stress and substrate behavior.

Experimental Validation: Core A is composed of Resin A and glass cloth, while Core B is composed of Resin B and glass cloth. These core materials A and B, each with distinct anisotropic resin properties as specified in Table V, were simulated and compared to experimental thermal shock test results. This case ensured that the simulation findings were consistent with the observed trends in crack formation.

Table V. Material properties of resin A and resin B

Material	CTE Anisotropy	In-plane CTE [ppm/K]
Resin A	1.8	66.1
Resin B	1.0	20.3

By integrating these simulations, the study effectively bridged macro-scale warpage effects and micro-scale stress mechanisms, offering detailed insights into the stress factors driving core cracking. This methodology provides an efficient framework for optimizing the material design of advanced semiconductor packages.

B. *Experimental Method*

To validate the simulation approach and its predictions, complementary experiments were conducted to assess both the thermal expansion characteristics and the crack initiation behavior of the composite core material. Comparative evaluations were performed for two core material variants, Core A and Core B, whose CTE anisotropy and absolute CTE values of resin are listed in Table V. To evaluate crack initiation, we fabricated test substrates mirroring the layer architecture adopted in the numerical model, with the chip size of 20 mm × 20 mm and the substrate size of 60 mm × 60 mm. We then examined crack formation after a thermal shock test. In this study, the liquid-to-liquid thermal shock test was conducted by alternately immersing the specimens in –65 °C and 120 °C baths for 500 cycles.

III. Results and Discussion

Generally, the CTE of the build-up layers and wiring layers is larger than that of the core. As a result, tensile stress in the out-of-plane direction occurs at the corners of the core during cooling. This study focuses on evaluating this stress.

The macro-scale simulation results indicated that adapting low CTE glass (Glass B) or a decrease in the resin's CTE lead to a corresponding increase in the in-plane CTE of the composite core, which reduces the out-of-plane tensile

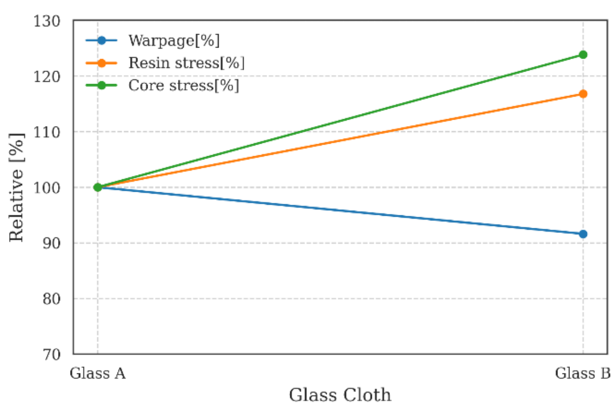

Fig. 4 Comparison of stress and warpage for different types of glass cloth based on simulation results. Values are normalized to 100% for Glass A as the reference.

stresses concentrated at the core's corner regions—a trend that is consistent with previous literature [12]. However, the reduction in core stress came at the cost of increased global substrate warpage, as evidenced by the FCBGA simulation results, shown in Fig. 4 and Fig. 5.

In the discussion of isotropic resin, the stress of the resin decreases when achieving a low CTE, which helps in suppressing warpage. However, in this case, the stress on the core increases, potentially leading to additional stress in regions other than those with a high resin content, such as at the resin–glass cloth interface. Therefore, there remains some doubt as to whether the trade-off has been completely resolved. For Anisotropic resin analysis, simulations were carried out with the resin's in-plane CTE fixed at 30 ppm/K; when the out-of-plane CTE of resin was adjusted to yield anisotropy of 1.0 and 2.0, the resulting local tensile stresses were found to be 90% and 110% of the baseline case (The

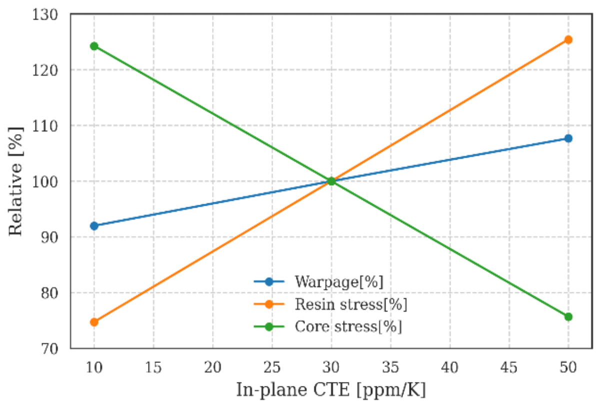

Fig. 5 Comparison of stress and warpage with isotropic resin based on simulation results. Values are normalized to 100% for the case where the resin's CTE is 30 ppm/K as the reference.

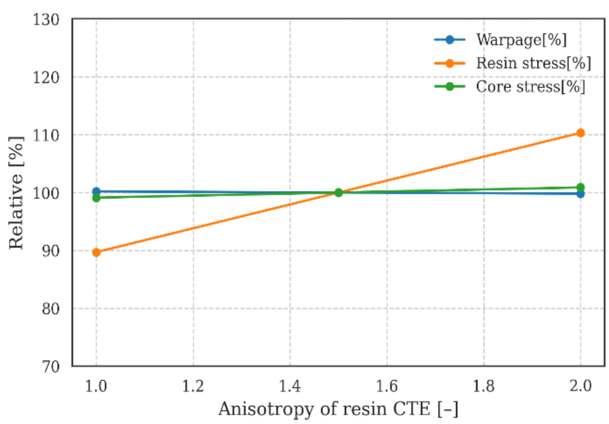

Fig. 6 Comparison of resin stress and warpage with anisotropic resin based on simulation results. Values are normalized to 100% for the resin with a CTE anisotropy of 1.5 as the reference.

100% stress reference is defined by the case with an anisotropy ratio of 1.5.) respectively. This suggests that reducing the resin's out-of-plane CTE helps minimize the contraction during cooling, thereby alleviating the tensile stresses responsible for initiating cracks. Notably, the simulations further show that modifying the resin's anisotropy has minimal impact on the overall board warpage and core stress (shown in Fig. 6), effectively decoupling the trade-off between crack suppression and warpage control.

Further investigation considered the resin as an anisotropic material. Experimental evaluation of the cores revealed that Core A exhibited a resin CTE anisotropy of approximately 1.8, whereas Core B demonstrated a value of approximately 1.0. The observed differences are considered to result from the combination and structure of the resin.

Complementary thermal shock tests reinforced these findings. After 500 cycles, the crack initiation rate for Core B was approximately 42% lower than that for Core A, shown in Table VI. Moreover, the simulation predicted a 45% reduction in localized core stress in Core B compared to Core A when identical elastic modulus was assumed. The agreement between the simulation and experimental results suggests that controlling the resin's through-thickness (out-of-plane) CTE relative to its in-plane CTE is a viable strategy for enhancing the reliability of semiconductor packages without incurring adverse effects on warpage.

Table VI. Simulated stress ratios and experimentally measured crack initiation rate ratios for core samples (values normalized to Core A = 1.00)

Material	Stress ratio by simulation	Crack Initiation Rate ratio by experiment
Core A	1.00	1.00
Core B	0.55	0.58

The results highlighted several critical points regarding stress management and warpage control in resin-based organic cores. First, the widely known approach of increasing the in-plane CTE of the core to reduce stress at free edge was found to be effective in decreasing core stress concentrations. However, this method also resulted in a significant increase in overall substrate warpage, presenting a major limitation for practical applications. In contrast, reducing the out-of-plane CTE of the resin offers a more promising alternative. This approach effectively suppresses corner local stress concentrations without negatively affecting the global warpage of the substrate and the stress of core. As a result, it enables the simultaneous achievement of crack suppression and warpage control, which are typically at odds with each other.

From a practical standpoint, it is challenging to achieve a resin CTE anisotropy ratio that is significantly smaller than 1.0. Therefore, maintaining the out-of-plane CTE of the resin close to its in-plane CTE (achieving a ratio near 1.0) emerges as a critical strategy for effective stress management and crack mitigation.

Finally, identifying new methods to significantly lower the resin's CTE anisotropy below 1.0 would have a substantial impact on crack suppression, particularly in the corner regions of the core. Such advancements could lead to breakthroughs in the reliability of semiconductor packages.

IV. CONCLUSION

In this study, we present a two-step multi-scale finite-element methodology to investigate and optimize the thermo-mechanical behavior of organic composite core materials used in advanced semiconductor packages. Homogenized anisotropic properties derived from representative volume elements were incorporated into macro-scale FCBGA models to capture global warpage and core-level stress, while micro-scale RVE analyses resolved local stress concentrations at free edge resin regions. The combined simulation and experimental results demonstrate that reducing the resin's out-of-plane CTE relative to its in-plane CTE, thereby minimizing the resin's CTE anisotropy, can substantially mitigate localized tensile stresses responsible for crack initiation at core corners, without producing appreciable increases in overall substrate warpage and core stress. Thermal-shock experiments corroborated the simulation trends, with cores featuring lower resin out-of-plane CTE showing markedly improved resistance to crack initiation. These findings provide practical design guidance: tailoring resin CTE anisotropy to minimize out-of-plane contraction is an effective route to suppress core cracking while preserving warpage control.

Consequently, the present conclusions are based on a stress-based relative assessment. In future work measured fracture toughness and interfacial properties should be considered to enable quantitative failure prediction and more rigorous material-to-material comparisons.

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