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A Multiscale Optimization Framework for Enhanced Warpage Control in Ceramic Substrates

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Abstract

In this study, a novel framework that integrates multiscale modelling and metaheuristic optimization is developed to minimize warpage in ceramic substrates used in microelectronics packaging. Ceramic substrates are prone to warpage due to the complex interactions between the ceramic microstructure and the heterogeneous circuit layout. To predict warpage accurately, effective ceramic material properties are derived using Laguerre–Voronoi tessellation combined with finite element-based homogenization, which captures the biphasic nature of sintered ceramics. A composite CAD model is generated to incorporate the substrate's hole features, and a volume-fraction-based homogenization method is applied to address the inhomogeneity between metallic and ceramic layers. To reduce computational effort, a surrogate model is trained on a multiscale warpage simulation dataset to predict the average vertical nodal displacement on the substrate's central plane under thermal loading. The optimal combination of design parameters that minimizes warpage is determined using the Teaching–Learning-Based Optimization (TLBO) algorithm. Validation against fine-scale simulations confirms that the proposed framework effectively predicts substrate warpage and identifies feasible, optimal design solutions.

Keywords: ceramic substrate, warpage, multiscale modelling, homogenization, surrogate model, finite element analysis, optimization.

1 Introduction

Ceramic substrate packaging is widely employed in the field of microelectronics packaging due to its exceptional thermal resistance and excellent electrical stability

[1]. However, manufacturing failures frequently occur due to warpage and the inherent mechanical durability limitations of ceramic materials. These challenges result in increased production costs and extended manufacturing periods. To address these issues, extensive research has been undertaken to elucidate and predict the relationships among factors such as substrate warpage, substrate thickness, process conditions, and via size [2,3]. Recent studies have increasingly focused on predicting warpage using surrogate models to optimize design parameters [4].

Accurate prediction of substrate warpage requires a precise estimation of the material properties constituting the substrate [5]. The properties of ceramics produced via the sintering process are predominantly determined by their microstructure; thus, Voronoi tessellation-based techniques have been proposed for effective modeling of polycrystalline ceramics [6,7,8]. These methods reliably capture the structural properties measured in experiments, thereby enhancing the accuracy of microstructural analyses.

Moreover, ceramics produced through sintering exhibit a biphasic structure, with different properties at grain boundaries compared to within the grains. This biphasic nature necessitates a homogenization process when applying the material data to macro-scale analyses. Various homogenization methodologies have been developed for multiscale analysis, including constructing Representative Volume Elements (RVEs) and extracting equivalent material properties via Finite Element (FE) analysis [9]. An alternative approach involves generating RVEs using Laguerre-Voronoi tessellation followed by applying the Voigt and Reuss models to obtain equivalent properties [10].

Constructing warpage analysis models becomes computationally demanding when fully accounting for the substrate's complex circuitry. Additionally, as the substrate is a multilayer structure composed of both insulating and metallic layers, it is critical to reflect the inhomogeneity of each layer. To overcome these challenges, composite micromechanics-based simplification methods have been proposed, enabling more efficient warpage analysis [11,12,13].

In this study, we introduce a comprehensive framework designed to facilitate the development of an optimal design and processing strategy for ceramic substrates. The framework integrates an equivalent material property modeling process that considers ceramic microstructure with a simplified warpage analysis model reflecting the substrate's circuit layout. Finally, we construct a multiscale warpage dataset to support the surrogate-based metaheuristic optimization framework to minimize warpage.

2 Methods

2.1 Overview of proposed framework

The proposed framework is designed to predict substrate warpage by simultaneously considering ceramic material properties based on ceramic microstructure and the heterogeneous distribution of metal and ceramic in the substrate macrostructure.

Based on this prediction, the framework seeks to determine the optimal parameter set that minimizes warpage.

The framework comprises three main processes:

1) multiscale warpage dataset generation,
2) surrogate model training,
3) metaheuristic optimization.

A conceptual diagram of the framework is presented in Figure 1.

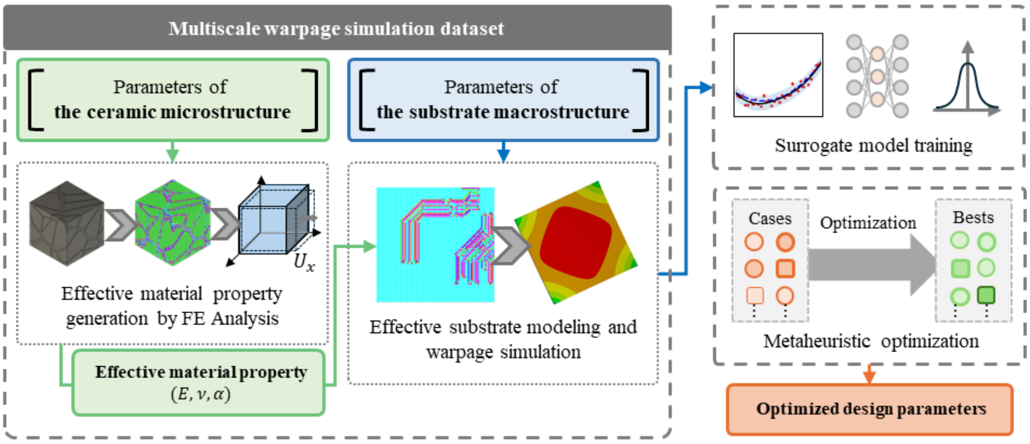

Figure 1: Conceptual diagram of ceramic substrate design optimization framework

First, ceramic material properties are estimated by generating the ceramic microstructure using Laguerre-Voronoi tessellation and applying the Voigt-Reuss assumptions to responses obtained from finite element analysis. Subsequently, a warpage analysis employing a simplification method is performed based on the estimated equivalent material properties and the substrate design parameters. The relationships between these factors and the warpage results are recorded in a multiscale warpage simulation dataset. This dataset is then used to train a surrogate model for rapidly predicting warpage outcomes. Various surrogate models are evaluated, and the most suitable one is selected through validation. The selected surrogate model is applied in a metaheuristic optimization process to obtain the optimal parameters that minimize warpage while accounting for multiscale effects.

2.2 Multiscale warpage dataset

2.2.1 Effective material properties generation

The Laguerre-Voronoi tessellation-based modelling approach combined with an FE-analysis-based homogenization technique is widely recognized as one of the most effective methods for capturing the characteristics of polycrystalline microstructures.

In this study, a polycrystalline microstructure without predefined boundaries is first generated using Laguerre-Voronoi tessellation, after which individual grains and grain boundaries are implemented through specific CAD operations applied to each grain.

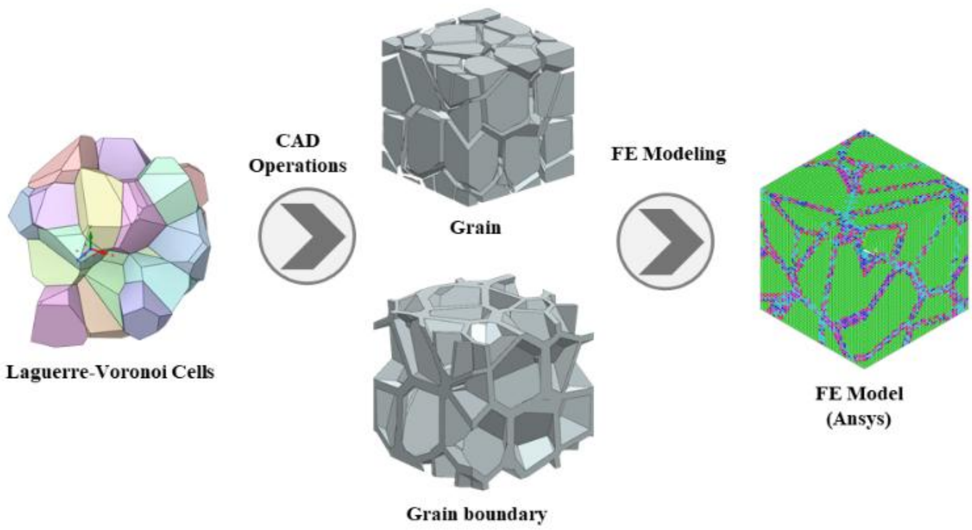

Figure 2: Workflow diagram of microstructure generation and corresponding FE model for homogenization

After randomly placing N grains within the unit cell, a Laguerre-Voronoi tessellation based on power distance is applied to partition the space. In this process, the radii of the spheres within the nuclei are sampled from a normal distribution defined by the mean and variance given as microstructure parameters. The formulations are as follows:

$$\{(\boldsymbol{\mathcal{X}}_{p_i}, r_i)\} = \{(\boldsymbol{\mathcal{X}}_{p_i}, r_i): \boldsymbol{\mathcal{X}}_{p_i} \sim U(0,1), r_i \sim \mathcal{N}(\mu, \sigma^2)\} \, \forall i \in \{1,2,\ldots,N\} \tag{1}$$

$$\{R_{P_i}\} = \{x \in R^3: |\boldsymbol{\mathcal{X}}_{p_i} - \boldsymbol{x}| - r_i^2 \leq |\boldsymbol{\mathcal{X}}_{p_j} - \boldsymbol{x}| - r_j^2\} \;\; \forall j \in \{1,2,\ldots,N\},\; j \neq i \tag{2}$$

To introduce boundary effects of the microstructure, geometric scaling-up and cut-off are applied between grain solids and their neighbours.

For the structural properties of the microstructure, tensile and shear loading conditions are applied in three different orientations, yielding a total of six cases, and the equivalent elastic modulus is subsequently calculated using the Voigt and Reuss models. Additionally, under the same framework, thermal properties are determined by evaluating the volumetric changes induced by variations in body temperature across three orientations, which allows for the computation of the coefficient of thermal expansion. All analyses and evaluations were performed using the Ansys Mechanical.

2.2.2 Effective substrate modeling and warpage simulation

A base CAD model incorporating the substrate's holes is generated by utilizing the substrate's macrostructural parameters. To perform a model simplification that accurately reflects the material property imbalance induced by the circuit layers and vias, a volume-fraction-based homogenization method is employed.

First, the circuit layer is modelled as a metal distributed on a plane based on actual circuit modelling data, while the vias are modelled as holes filled with metal. Subsequently, the volume-fraction-based homogenization method is applied to the mesh generated from the base CAD model. By incorporating the previously determined equivalent ceramic properties and the specified properties of the metal paste, a simplified model with low computational cost is achieved.

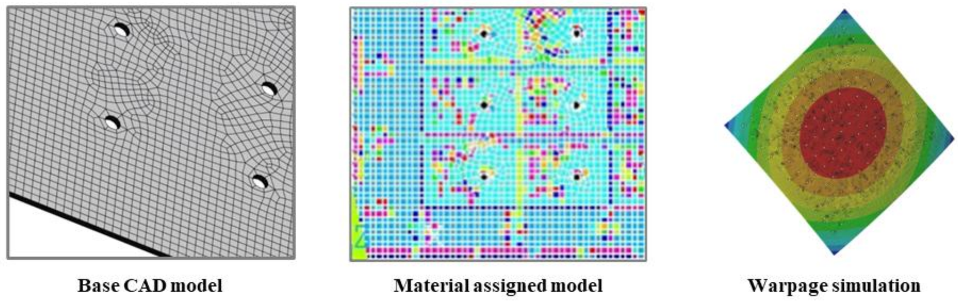

Figure 3: Material assigned model and visualized warpage simulation result.

2.3 Surrogate model training

Direct modification of the model, subsequent analyses, and evaluation of outcomes due to changes in the optimization design parameters incur a tremendous computational cost. Therefore, to accelerate the overall process of modelling, analysis, and result extraction, a surrogate model was developed using the multiscale warpage dataset generated in previous steps. This model is designed to predict the average vertical nodal displacement on the substrate’s central plane under thermal loading, based on the input parameters. To achieve the most accurate predictions, training was conducted using three different methods: Radial Basis Function, Multi-Layer Perceptron, and Gaussian Process Regression and their performance was evaluated via leave-one-out cross validation. The model demonstrating the best performance was then adopted.

2.4 Metaheuristic optimization

To determine the optimal combination of parameters that minimizes substrate warpage, an optimization problem was formulated.

$$objective\ function: min(\overline{u_z}),\ \overline{u_z} = \frac{1}{N}\sum_{i=1}^{N} u_{z,i} \qquad (3)$$

The value of the objective function of a design set is computed using the surrogate outputs.

In this study, the Teaching-Learning-Based Optimization (TLBO) algorithm, a metaheuristic method, was utilized to explore new designs. It draws inspiration from the dynamics of teaching and learning processes observed in classroom settings [14]. As a population-based approach, TLBO iteratively refines a group of candidate solutions to reach the global optimum. Unlike other methods, TLBO's performance is influenced solely by the size of its search population.

3 Results

To validate the proposed framework, we evaluated the warpage accuracy of the equivalent substrate model as well as the maximum accuracy of each surrogate model.

In verifying the warpage accuracy of the effective substrate model, the fine model reflecting the actual circuit geometry was regarded as the exact solution, and the error between the equivalent and fine models was determined. The detailed formulation of the Weighted Mean Absolute Percentage Error (WMAPE) and the error between the two models is provided as follows.

$$\text{WMAPE} = \frac{\sum_{i=1}^{n} | y_i - \hat{y}_i |}{\sum_{i=1}^{n} | y_i |} \times 100\% \tag{4}$$

	Case A	Case B
WMAPE	19.06%	14.88%

Table 1: WMAPE between warpage of effective substrate model and fine model

To assess the accuracy of each surrogate model, we trained the models using the Multiscale Warpage dataset generated from preset parameters and compared the resulting predictions. A train/test split was applied, and the model selected through leave-one-out cross validation on the training set was subsequently evaluated on the test set.

$$\text{MAPE} = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{y_i - \hat{y}_i}{y_i} \right| \times 100\% \tag{5}$$

	RBF	MLP	GPR
MAPE	8.41%	9.82%	9.41%

Table 2: The test set Mean Absolute Percentage Error (MAPE) for the three surrogates

4 Conclusions and Contributions

In this study, both the micro-level parameters determining the ceramic properties from sintering and the macro-level parameters inducing substrate deformation during thermal processing were considered. Ultimately, a metaheuristic-based optimization framework was proposed to explore the optimal parameters at each level that can suppress substrate warpage. Each component of the framework was validated in terms of performance and feasibility, ensuring that the optimization results are practical.

Furthermore, by training various surrogate models and selecting the best-performing one, a model that accurately replicates the multiscale analysis results of the substrate was developed. Consequently, the combined surrogate model and metaheuristic optimization approach demonstrates that a fast and efficient exploration of optimal design parameters at the early stages of substrate design is achievable.

Acknowledgements

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