

## Full Length Article

## Graded infill design of thin-walled structures with connectable nonuniform microstructures based on the data-driven surrogate model

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## ABSTRACT

This paper proposes a structural optimization framework for the high-performance and lightweight design of curved thin-shell structures. The proposed method integrates conformal mapping, a parameterized level-set method (PLSM), and a Kriging-based surrogate modeling strategy to obtain the graded infill design of thin-walled structures. At the macroscopic level, conformal mapping is employed to project the original three-dimensional (3D) curved surface onto a two-dimensional (2D) parametric domain, thereby reducing the dimension of the design problem. At the microscopic level, PLSM is introduced to define multiple prototype microstructures with diverse geometric features. A shape interpolation method is then developed to map these prototypes into a family of nonuniform microstructures. To reduce the computational burden, these microstructures serve as sample points to construct a Kriging metamodel for efficient property prediction. Through a mapping-design-inverse mapping process, the optimized graded microstructures are precisely projected back onto the original 3D surface while preserving geometric fidelity. The objective function is to minimize structural compliance subject to a global volume constraint. Sensitivity analysis formulas are derived based on a conformal thin-shell finite element model and PLSM, and expansion coefficients of the prototype microstructures are updated using the Optimality Criteria (OC) method. The effectiveness of the proposed framework is demonstrated through two examples: a vase shell and a turbine blade shell.

## 1. Introduction

Thin-walled and curved shell structures are extensively utilized in aerospace [1,2], automotive [3], and marine engineering [4,5] due to their high strength-to-weight ratio. In recent years, with the rapid advancement of Additive Manufacturing (AM) [6,7] technologies, it has become feasible to fabricate such structures with embedded cellular infills or metamaterials, opening new opportunities for lightweight design. To further reduce weight while maintaining or even enhancing mechanical performance, replacing solid materials within thin-walled structures with porous [8] or lattice [9,10] infills has emerged as a promising strategy. Compared with uniform infill patterns, functionally graded nonuniform infills [11,12] can tailor the local material distribution to specific load paths, offering superior structural stiffness, energy absorption, and thermal management capabilities.

To achieve the optimal design of these graded infills, a theoretical

framework via topology optimization based on Solid Isotropic Material with Penalization (SIMP) [13,14], Level-Set Methods (LSM) [15,16], and Moving Morphable Component (MMC) [17] method has been applied to the design of multiscale structures. Among various strategies, a number of approaches have been developed to enhance the accuracy, manufacturability, and the computational efficiency of shell-structure design. Ji et al. [13] proposed a parameter-free concurrent shape and topology optimization method using a two-step anisotropic-isotropic filtering and projection scheme. It enables uniform thickness control for stamping thin-walled structures. Li et al. [14] further improved this filtering framework by optimizing the length scale parameter of a Helmholtz-type PDE filter, allowing spatially varying filtering strength to achieve non-uniform interface thickness in multiple lattice materials. Zhu et al. [18] proposed a particle-flow topology optimization method based on a Lagrangian-Eulerian hybrid formulation, which effectively avoids localized geometric hinges in compliant mechanism design.

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Zhang et al. [19] developed an aerodynamic topology optimization framework for shell structures by combining a T-splines-based panel method with isogeometric analysis. Gao et al. [20] presented a multi-patch isogeometric topology optimization method that handles non-conforming meshes via Nitsche's method for periodic and graded cellular structures. Lin et al. [21] extended the particle-flow approach in a Lagrangian-Eulerian description using an isogeometric material point method to maximize structural loading-capability. Isogeometric analysis (IGA) has also been introduced into multiscale topology optimization. Liu et al. [16] combined IGA with the SIMP method and decoupled sensitivity analysis, developing a multi-objective framework to simultaneously achieve high thermal conductivity and low mechanical compliance.

Despite these advances, most existing methods are limited to planar domains or simple regular geometries. For curved surfaces, Xing et al. [22] and Ding et al. [23] applied conformal mapping to shell structures analysis. Zhang et al. [24] and Xu et al. [25] developed a NURBS-based parameterization framework for topology optimization on curved domains. However, these works focused on macroscopic shell optimization and did not consider graded infill design at the microscale. The extension to curved thin-shell surfaces with graded, connectable nonuniform microstructures remains challenging.

Two major computational issues arise. First, direct 3D multi-scale topology optimization of curved shell structures requires an enormous number of finite elements to capture both the macroscopic curvature and microscopic details, leading to a prohibitive computational burden. Second, in a multiscale topology optimization scheme, continuously updating the geometries and re-evaluating their homogenized properties at each iteration introduces substantial computational overhead.

To address these computational challenges, surrogate modeling has been widely adopted to accelerate the multiscale optimization. Various surrogate modeling and interpolation have been developed and applied in this context, each with its own strengths and limitations. Wang et al. [26,27] proposed a framework that combines parameterized microstructure libraries with polynomial interpolation for rapid property mapping. This approach is computationally efficient but may struggle to accurately capture highly non-linear relationships between microstructure geometry and effective properties, especially when the design space is large. Recently, machine learning-based approaches have also emerged to address these computational challenges. For instance, a Bayesian optimization framework combined with Triply Periodic Minimal Surfaces (TPMS) has been proposed by Wu et al. [28] for functionally graded ceramic scaffolds, achieving enhanced biomechanical performance at low computational cost. Similarly, a derivative-aware machine learning algorithm has been developed for multiscale topology optimization of nonuniform lattice structures to achieve uniform strain distribution [29]. White et al. [30] and Luo et al. [31] employed deep neural networks (DNNs) [32,33] for high-precision performance prediction and graded microstructure design. DNNs are capable of learning complex, nonlinear mappings from training data and have demonstrated excellent accuracy in many applications. However, they typically require a large amount of training data, which can be expensive to generate via numerical homogenization. Additionally, the training process itself is computationally intensive, and the resulting models may lack interpretability. Zheng et al. [34] introduced a Kriging-based multiscale optimization method combined with smooth evolutionary strategies for efficient design of hierarchical structures. Kriging offers several advantages, including the ability to provide both predictions and uncertainty estimates, as well as good performance with relatively small training datasets.

To bridge the research gap, this paper proposes a data-driven structural optimization framework based on the Kriging model for the high-performance and lightweight design of curved thin-shell structures with connectable nonuniform microstructures. Instead of direct 3D

optimization, a mapping-design-inverse mapping strategy is adopted. Conformal mapping is utilized to project the 3D curved surface onto a 2D parametric domain, preserving local angles exactly and minimizing geometric distortion. A set of representative microstructural prototypes is first defined. At the microscopic level, a parameterized level-set method combined with a shape interpolation scheme is then developed to map these prototypes into a continuous family of nonuniform microstructures that share similar topological features, guaranteeing connectivity between adjacent cells. To further eliminate the computational bottleneck without sacrificing accuracy, a data-driven surrogate model based on the Kriging model is introduced. The PLSM-generated microstructures are used to construct a Kriging metamodel, which effectively and accurately predicts equivalent material properties during the optimization process. Utilizing the Optimality Criteria method and sensitivity analysis based on a conformal thin-shell finite element model, the structural compliance is minimized under a global volume constraint.

The main contributions of this study are summarized as follows:

- (1) A dimensionality-reduction framework combining conformal mapping and PLSM shape interpolation is proposed. It enables the design of geometrically faithful and connected graded microstructures on complex 3D curved shells.
- (2) A Kriging-driven learning strategy is integrated into the multi-scale topology optimization loop, drastically reducing the number of costly homogenization evaluations required during optimization, while maintaining high accuracy in predicting the elastic property.

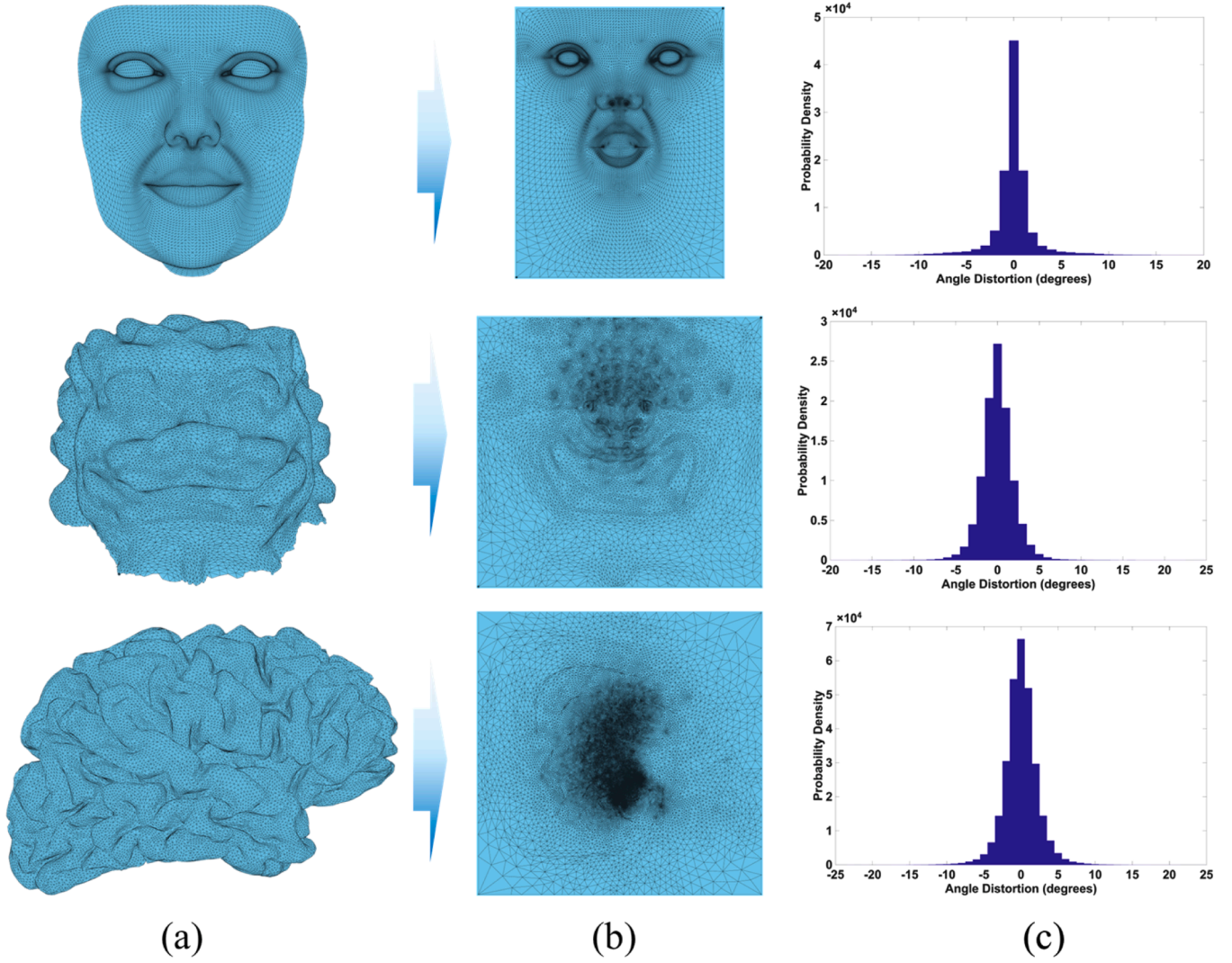
The remainder of this paper is organized as follows: Section 2 introduces the conformal mapping process and the corresponding thin-shell finite element model, laying the theoretical foundation for the dimensionality-reduced design of curved shell structures. Section 3 elaborates on the generation of connectable nonuniform microstructures using the PLSM, the construction of the Kriging metamodel for efficient property prediction, the formulation of the multiscale topology optimization problem, and the derivation of sensitivity analysis formulas. Section 4 presents the numerical implementation details of the proposed optimization framework, including the workflow and convergence criteria. Section 5 demonstrates the effectiveness of the framework through two representative examples: a vase shell and turbine blade shell numerical example, and further verifies the optimization performance by comparing different infill types and uniform infill designs. Finally, conclusions and future work are drawn in Section 6. To improve clarity and help readers easily identify the meaning of each symbol, a Nomenclature section is presented in Appendix A.

## 2. Conformal geometry-based parametric representation of free-form surfaces

Conformal geometry provides a theoretical foundation for mapping complex free-form surfaces onto canonical parametric domains [35]. A central concept is the conformal mapping, also known as an angle-preserving map [36]. As illustrated in Fig. 1, for any point on the free-form surface, the angle between two arbitrary vectors originating from this point before conformal mapping should remain equal to the angle between their corresponding vectors after mapping. This property ensures that the local shape of the surface is preserved during the transformation.

To facilitate a better understanding for the reader, the basic conformal mapping theory is illustrated briefly. Let  $M_1$  and  $M_2$  denote two Riemannian surfaces with the local coordinate system  $r_1(x^1, x^2)$  and  $r_2(x^1, x^2)$ . The first fundamental forms of  $M_1$  and  $M_2$  are given by [37]:





**Fig. 1.** Illustration of conformal mapping for free-form surfaces of the human face, lion, and brain. (a) Original surface, (b) Parameter domain after conformal mapping, (c) Angle distortion.

$$ds_1^2 = \sum_{ij} g_{ij} dx^i dx^j \quad (1)$$

$$ds_2^2 = \sum_{ij} \tilde{g}_{ij} dx^i dx^j \quad (2)$$

where

$$g_{ij} = \frac{\partial r_1}{\partial x^i} \frac{\partial r_1}{\partial x^j}, \tilde{g}_{ij} = \frac{\partial r_2}{\partial x^i} \frac{\partial r_2}{\partial x^j}, i, j = 1, 2 \quad (3)$$

Here,  $ds_1^2$  and  $ds_2^2$  denote the squared infinitesimal arc elements on  $M_1$  and  $M_2$ . Through the mapping  $f: M_1 \rightarrow M_2$ , any vector on  $M_1$  can be mapped to  $M_2$ . The mapping  $f = (f^1(x^1, x^2), f^2(x^1, x^2))$  then satisfies the following relationship:

$$\begin{pmatrix} df^1 \\ df^2 \end{pmatrix} = \begin{pmatrix} \frac{\partial f^1}{\partial x^1} & \frac{\partial f^1}{\partial x^2} \\ \frac{\partial f^2}{\partial x^1} & \frac{\partial f^2}{\partial x^2} \end{pmatrix} \begin{pmatrix} dx^1 \\ dx^2 \end{pmatrix} \quad (4)$$

The length of  $df$  is:

$$df = \sum_{m,n} g_{mn} df^m df^n \quad (5)$$

By replacing  $dfm$  in Eq. (5) by Eq. (4), the analytical formulation of the new metric for  $M_1$ , induced by the mapping  $f$  and the metric on  $M_2$ , is given by:

$$f^* ds_2^2 = \sum_{mn} \left( \sum_{ij} \tilde{g}_{ij} (f(x_1, x_2)) \frac{\partial f^m}{\partial x_i} \frac{\partial f^n}{\partial x_j} \right) dx^m dx^n \quad (6)$$

where  $f$  is a conformal mapping, meaning there exists a positive conformal factor  $\lambda(x_1, x_2)$  such that the metric satisfies  $f^* ds_2^2 = \lambda(x_1, x_2) ds_1^2$ .

Based on the uniformization theorem [38], a shell structure can be conformally mapped to the 2D parametric plane. The optimized graded infill design is then mapped back onto the original shell surface via the inverse conformal transformation  $(x, y, z) = f^{-1}(u, v)$ , where  $(u, v)$  is the orthogonal curvilinear coordinate system. This streamlined workflow, termed the Map-Design-Inverse process, simplifies the design of lattice metamaterials on free-form surfaces. By reducing the dimensionality of the design problem, it effectively bridges the gap between design simplicity and geometric complexity.

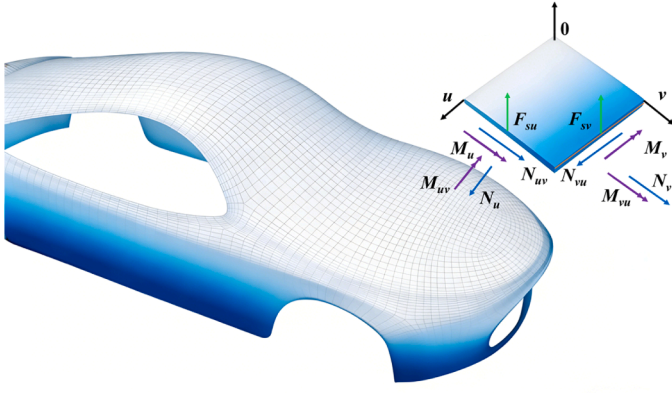


Fig. 2. Illustration of a shell element in a vehicle body with typical parameters.

The conformal shell finite element analysis is derived to calculate physical responses defined in the parametric space  $(u, v)$ . As illustrated in Fig. 2, the geometric equations of the shell structure are given by [39]:

$$\begin{cases} \epsilon_u = \epsilon_u + \chi_u \tau \\ \epsilon_v = \epsilon_v + \chi_v \tau \\ \epsilon_{uv} = \epsilon_{uv} + \chi_{uv} \tau \end{cases} \quad (7)$$

where  $\tau$  denotes the normal distance from an arbitrary point  $P$  on the conformal shell to the mid-surface,  $\epsilon_u$  and  $\epsilon_v$  are the normal strains,  $\epsilon_{uv}$  is the shear strain,  $\chi_u$  and  $\chi_v$  are the changes in principal curvatures  $k_1$  and  $k_2$  along  $u$ - and  $v$ -directions, respectively, and  $\chi_{uv}$  is the twist rate along  $u$ - and  $v$ -directions. They satisfy the following equations:

$$\begin{cases} \epsilon_u = \frac{1}{A} \frac{\partial v}{\partial u} + \frac{1}{AB} \frac{\partial A}{\partial v} v + k_1 \omega \\ \epsilon_v = \frac{1}{B} \frac{\partial v}{\partial v} + \frac{1}{AB} \frac{\partial B}{\partial u} v + k_2 \omega \\ \epsilon_{uv} = \frac{A}{B} \frac{\partial}{\partial v} \left( \frac{v}{A} \right) + \frac{B}{A} \frac{\partial}{\partial u} \left( \frac{v}{B} \right) \\ \chi_u = -\frac{1}{A} \frac{\partial}{\partial u} \left( \frac{1}{A} \frac{\partial \omega}{\partial u} \right) - \frac{1}{AB^2} \frac{\partial A}{\partial v} \frac{\partial \omega}{\partial v} \\ \chi_v = -\frac{1}{B} \frac{\partial}{\partial v} \left( \frac{1}{B} \frac{\partial \omega}{\partial v} \right) - \frac{1}{A^2 B} \frac{\partial B}{\partial u} \frac{\partial \omega}{\partial u} \\ \chi_{uv} = -\frac{1}{AB} \left( \frac{\partial^2 \omega}{\partial u \partial v} - \frac{1}{A} \frac{\partial A}{\partial v} \frac{\partial \omega}{\partial u} - \frac{1}{B} \frac{\partial B}{\partial u} \frac{\partial \omega}{\partial v} \right) \end{cases} \quad (8)$$

where  $A$  and  $B$  are the Lamé coefficients along  $u$ - and  $v$ -directions, respectively. The Lamé coefficients on the conformal shell at distance  $\tau$  from the mid-surface are given by:  $H_1 = A(1 + k_1 \tau)$  and  $H_2 = B(1 + k_2 \tau)$ , and  $\omega$  denotes the deflection along the direction normal to the mid-surface.

Assuming a linear elastic material and neglecting transverse shear forces, the physical equations can be written in matrix form as:

$$\begin{bmatrix} N_u \\ N_v \\ N_{uv} \\ M_u \\ M_v \\ M_{uv} \end{bmatrix} = \frac{ET}{1-\mu^2} \begin{bmatrix} \mu & 1 & 0 & 0 & 0 & 0 \\ 1 & \mu & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1-\mu}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{T^2}{12} & \frac{T^2 \mu}{12} & 0 \\ 0 & 0 & 0 & \frac{T^2 \mu}{12} & \frac{T^2}{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{T^2(1-\mu)}{24} \end{bmatrix} \begin{bmatrix} \epsilon_u \\ \epsilon_v \\ \epsilon_{uv} \\ \chi_u \\ \chi_v \\ \chi_{uv} \end{bmatrix} \quad (9)$$

where  $E$  is the Young's modulus,  $\mu$  is the Poisson's ratio, and  $T$  is the thickness of the conformal shell. The constitutive equations of thin-

walled structures can be written in matrix form as:

$$D = \frac{ET}{1-\mu^2} \begin{bmatrix} \mu & 1 & 0 & 0 & 0 & 0 \\ 1 & \mu & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1-\mu}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{T^2}{12} & \frac{T^2 \mu}{12} & 0 \\ 0 & 0 & 0 & \frac{T^2 \mu}{12} & \frac{T^2}{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{T^2(1-\mu)}{12 \cdot 2} \end{bmatrix} \quad (10)$$

Following the classical shell theory, the equivalent matrix of elasticity coefficients can be further decomposed into two distinct components:  $\sigma^{(m)} = D^{(m)} \epsilon^{(m)}$  and  $\sigma^{(b)} = D^{(b)} \epsilon^{(b)}$  [36]. They describe the thin plate state and bending state of the shell structure, respectively. It is noted that they have the following relationship:  $D^{(b)} = \frac{T^2}{12} D^{(m)}$ . Finally, the strain energy  $J$  of the shell structures is given by :

$$J = \frac{1}{2} \int_{\Omega} (\epsilon^{(m)})^T D^{(m)} \epsilon^{(m)} d\Omega + \frac{1}{2} \int_{\Omega} (\epsilon^{(b)})^T D^{(b)} \epsilon^{(b)} d\Omega \quad (11)$$

This energy formulation serves as the basis for the compliance minimization in the subsequent topology optimization. Additionally, to avoid redundancy in the numerical homogenization method in Section 3,  $D^{(b)}$  and  $D^{(m)}$  are both denoted as  $D^{(*)}$ .

### 3. Kriging-assisted mechanical model for the graded microstructures

In this work, graded microstructures that vary with spatial distribution are considered. However, it introduces a substantial increase in computational cost because conventional multiscale topology optimization relies on iterative finite element analysis and a homogenization method to compute the equivalent elasticity tensor for each microstructure candidate. Thus, this work establishes an efficient Kriging-assisted mechanical model to bridge this gap by establishing an explicit mapping between the effective density and the equivalent elasticity tensor of graded microstructures.

#### 3.1. Connectable infill microstructures with local level sets

The parametric level-set method (PLSM) [40,41] is a numerical technique that implicitly represents a moving boundary as the zero level set of a higher-dimensional function, which allows it to naturally handle topological changes without reparameterization, as shown in Fig. 3. Firstly, we define a prototype microstructure based on a level-set function. The specific form of the level-set function is given as:

$$\begin{cases} \Phi(x) > 0, \forall x \in \Omega \setminus \partial\Omega(\text{Solid}) \\ \Phi(x) = 0, \forall x \in \Omega(\text{Boundary}) \\ \Phi(x) < 0, \forall x \in \text{Domain} \setminus \partial\Omega(\text{Void}) \end{cases} \quad (12)$$

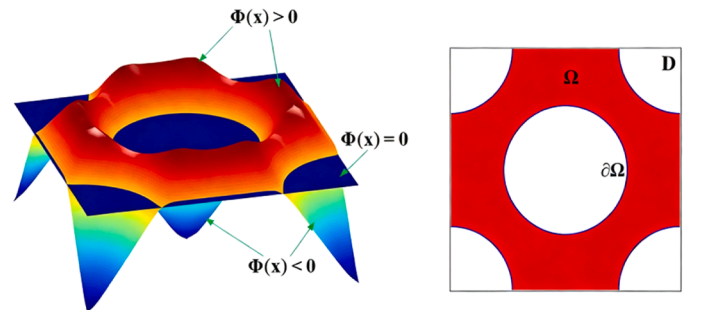


Fig. 3. Level-set boundary representation of a prototype microstructure [42].

where  $\Omega$  denotes the set of all admissible shapes for non-uniform microstructures,  $\partial\Omega$  is the structural boundary of the prototype microstructure, and  $x$  is the spatial coordinates.

Subsequently, a set of graded microstructures can be generated by interpolating the level-set function of the prototype microstructure. The interpolation formula is given as:

$$\Phi_e(x) = \Phi(x) + \varphi_e, \quad (e = 1, 2, \dots, ne) \quad (13)$$

where  $\varphi_e \in [\min(\Phi), \max(\Phi)]$  represents the shape interpolation coefficient,  $ne$  is the total number of microstructures. As shown in Fig. 4, these microstructures share similar topological features, thereby ensuring connectivity among adjacent units. The interpolation is restricted to a practical density sub-interval, rather than the full range  $\rho \in [0, 1]$ . A lower bound  $f_{pm}$ , which is set to 0.1 in this work, is introduced to avoid the occurrence of void regions [43–45]. The effective density of the  $e$ -th graded microstructure obtained by interpolating the  $m$ -th prototype, which is expressed as follows:

$$\rho_{m,e} = \frac{1}{|\Omega_{m,e}|} \int_{\Omega_{m,e}} d\Omega_{m,e} \quad (14)$$

The PLSM framework is capable of generating a much wider variety of irregular microstructures. Additional microstructures are provided in Fig. 5 to demonstrate the geometric flexibility of the level-set representation. However, the present optimization study focuses on the three prototype families shown in Fig. 4. Interested readers may explore other microstructure configurations using the same framework.

The graded microstructures are tailored to achieve a prescribed sequence of effective densities. To this end, a bi-section algorithm [42] is employed to iteratively determine the shape interpolation coefficients that yield microstructures with the target densities. The pseudocode in Algorithm 1 gives an idea to solve the shape interpolation coefficient for graded microstructures, which aims to obtain the optimal interpolation coefficient that makes the effective density of the generated graded microstructure consistent with the target effective density while ensuring the geometric connectivity of the microstructure.

It can be seen that the bisection method [46,47] is employed as an outer loop. Starting with an initial bracket  $[\varphi_{\min}, \varphi_{\max}]$ , the algorithm iteratively evaluates the microstructure geometry for the midpoint

threshold  $\rho(\Phi(x) - \varphi_{\text{mid}})$ , narrows the bracket based on the sign of the error between the achieved and target densities, and continues until the relative error is reduced below a strict tolerance, typically set to 0.01%.

**Algorithm 1.** Solve shape interpolation coefficient.

---

**Input:**  $m, \rho, \varphi_{\min}, \varphi_{\max}, \Phi(x), \varepsilon, \text{maxiter}$

```

1  Iter=0;
2  while (Iter < maxiter) and ( $|\rho_e - \rho| > \varepsilon$ ) do
3       $\varphi_{\text{mid}} = (\varphi_{\min} + \varphi_{\max}) / 2$ ;
4       $\Phi_e = \Phi - \varphi_{\text{mid}}$ ;
5      Calculate the effective density  $\rho_e$  of  $\Phi_e$  in Eq.(14);
6      if  $\rho_e < \rho$  then
7           $\varphi_{\min} = \varphi_{\text{mid}}$ ;
8      else if  $\rho_e > \rho$  then
9           $\varphi_{\max} = \varphi_{\text{mid}}$ ;
10     else
11         break
12     end if
13     iter=iter+1;
14 end while
15  $\varphi_e = \varphi_{\text{mid}}$ ;

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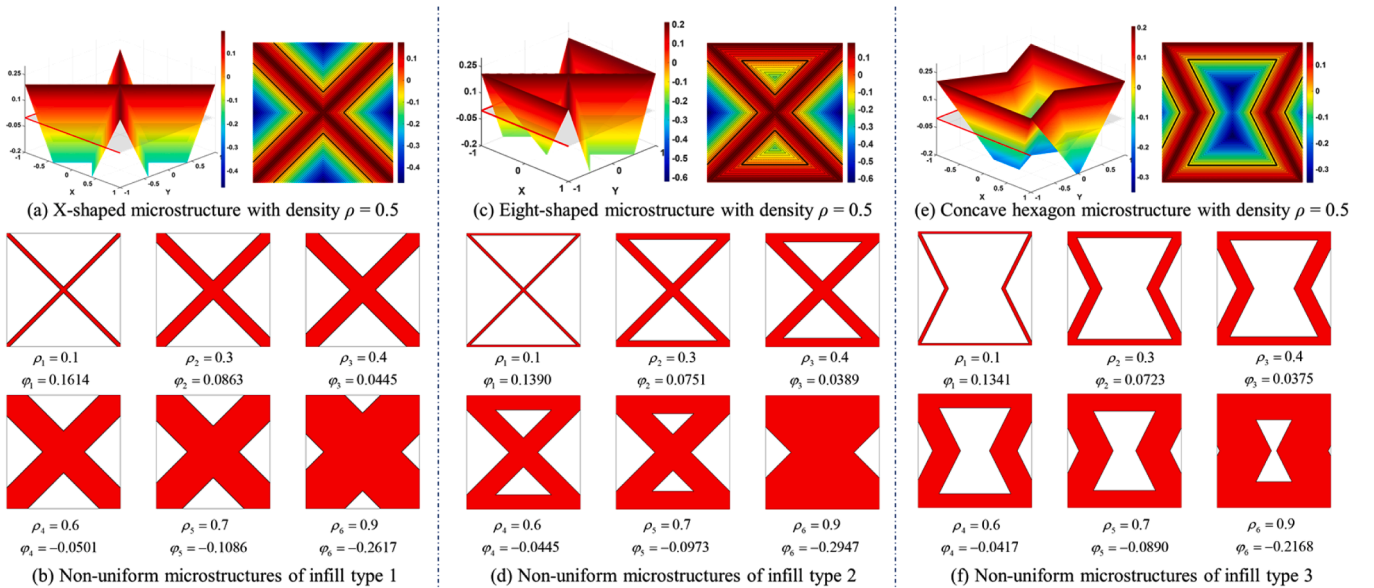
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**Output:**  $\varphi_e$

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### 3.2. Efficient prediction of equivalent properties for graded microstructures based on the data-driven surrogate model

Kriging models are widely employed in aerospace, automotive, and electronics industries for surrogate modeling to reduce computational costs [48–50]. To construct a Kriging predictor for equivalent properties, a set of microstructure samples is generated by interpolating the prototype within the target density sub-interval. Once the level-set functions defining the microstructural geometries are available, their effective elastic tensors are computed using a numerical homogenization method [51,52], which is given by:



**Fig. 4.** Three structurally distinct prototype microstructures including X-shaped, eight-shaped and concave hexagon-shaped and their corresponding families of graded microstructures generated by the threshold shifting, together with the equivalent densities and shape interpolation coefficients.



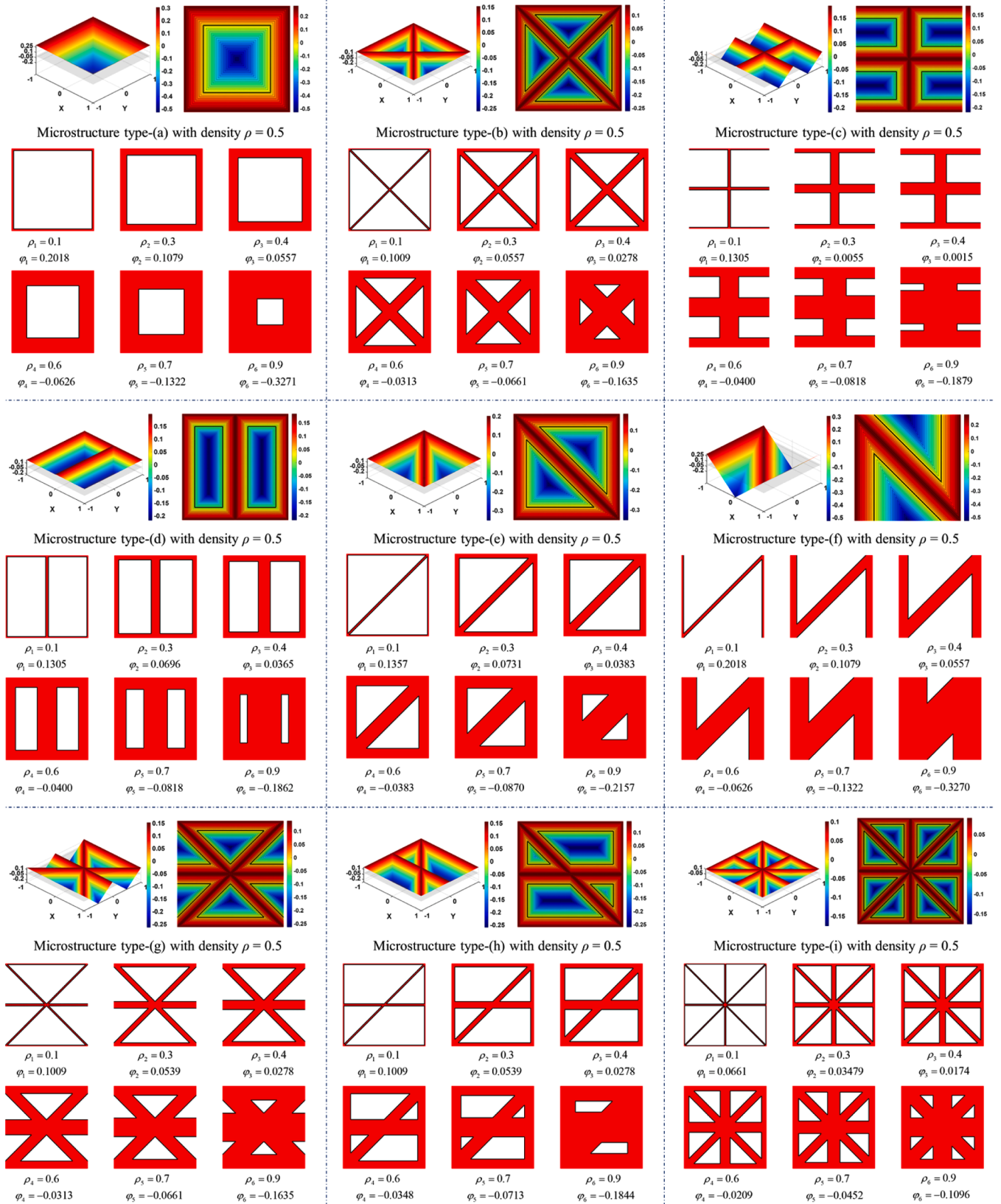


Fig. 5. Additional PLSM-generated microstructure examples, demonstrating the geometric flexibility of the level-set representation beyond the three prototype families used in the main optimization.



$$\left(\mathbf{D}_{ijkl}^H\right)_{m,e} = \frac{1}{|\Omega_{m,e}|} \int_{\Omega_{m,e}} \left( \varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^* \left( \mathbf{u}_{m,e}^{(ij)} \right) \right) \mathbf{D}^{(m)} \left( \varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^* \left( \mathbf{u}_{m,e}^{(kl)} \right) \right) H(\Phi_{m,e}) d\Omega_{m,e} \quad (15)$$

where  $i, j, k, l = 1, 2, \dots, d$  is the spatial dimension,  $H(\Phi_{m,e})$  is the Heaviside function distinguishing solid and void phases,  $\varepsilon_{pq}^{0(ij)}$  is the prescribed macroscopic test strain field,  $\varepsilon_{pq}^* \left( \mathbf{u}_{m,e}^{(ij)} \right)$  is the microscopic local strain field, and the microscopic displacement field  $\mathbf{u}_{m,e}^{(ij)}$  is obtained by solving the linear elastic equilibrium equation, which is given by:

$$\int_{\Omega_{m,e}} \left( \varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^* \left( \mathbf{u}_{m,e}^{(ij)} \right) \right) \mathbf{D}^{(m)} \varepsilon_{rs}^* \left( \mathbf{v}_{m,e}^{(kl)} \right) H(\Phi_{m,e}) d\Omega_{m,e} = 0, \forall \mathbf{v}_{m,e}^{(kl)} \in \bar{\mathbf{U}}(\Omega_{m,e}) \quad (16)$$

where  $\mathbf{v}_{m,e}^{(kl)}$  is the virtual displacement field, and  $\bar{\mathbf{U}}(\Omega_{m,e})$  is the kinematically admissible periodic displacement field. The periodic boundary conditions (BC) can be referred to literature [53].

The Kriging model combines a global regression model with a localized stochastic process, which is given by:

$$\mathbf{D}^H(\rho^{MA}) = \mathbf{f}(\rho^{MA})^T \boldsymbol{\beta} + \mathbf{Z}(\rho^{MA}) \quad (17)$$

where  $\mathbf{D}^H(\rho^{MA})$  is the predicted response at the prediction point  $\rho^{MA}$ ,  $\mathbf{f}(\rho^{MA})$  is a  $ne \times 1$  vector of known basis functions of regression functions,  $\boldsymbol{\beta}$  is a vector of corresponding regression coefficients, and  $\mathbf{Z}(\rho^{MA})$  is a Gaussian random process with zero mean and variance  $\sigma_z^2$ . Based on unbiased estimation prediction, the mean squared error at the predicted point is given by:

$$\hat{\sigma}_{\hat{\mathbf{D}}^H}^2(\rho^{MA}) = \hat{\sigma}_z^2 \left[ 1 + \mathbf{u}^T (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} \mathbf{u} - \mathbf{r}(\rho^{MA})^T \mathbf{R}^{-1} \mathbf{r}(\rho^{MA}) \right] \quad (18)$$

where  $\mathbf{u} = \mathbf{F}^T \mathbf{R}^{-1} \mathbf{r}(\rho^{MA}) - \mathbf{f}(\rho^{MA})$ ,  $\mathbf{R}$  is a  $ne \times ne$  correlation matrix,  $\mathbf{Y}$  is the true response at the training points,  $\hat{\boldsymbol{\beta}}$  is the generalized least square estimator of  $\boldsymbol{\beta}$ ,  $\mathbf{r}(\rho^{MA})$  is the correlation vector between the untried points  $\rho^{MA}$  and each of the  $ne$  training points. They are expressed by:

$$\hat{\boldsymbol{\beta}} = (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{R}^{-1} \mathbf{Y} \quad (19)$$

$$\mathbf{r}(\rho^{MA}) = [\mathbf{R}(\rho^{MA}, \rho_1^{MA}; \boldsymbol{\theta}), \mathbf{R}(\rho^{MA}, \rho_2^{MA}; \boldsymbol{\theta}), \dots, \mathbf{R}(\rho^{MA}, \rho_{ne}^{MA}; \boldsymbol{\theta})]^T \quad (20)$$

The hyper-parameter  $\boldsymbol{\theta}$  is determined by maximizing the likelihood function, leading to the following unconstrained optimization problem:

$$\max : L(\boldsymbol{\theta}) = - (ne \ln(\hat{\sigma}_z^2) + \ln[|\mathbf{R}|]) \quad (21)$$

Once trained, the response of predicted points is subjected to a normal distribution:

$$\hat{\mathbf{D}}^H \sim N(\hat{\mathbf{D}}^H(\rho^{MA}), \hat{\sigma}_{\hat{\mathbf{D}}^H}^2(\rho^{MA})) \quad (22)$$

Accordingly, the effective elastic properties can be effectively predicted via the Kriging prediction model associated with its corresponding prototype:

$$\mathbf{D}_{ijkl}^H(\rho^{MA}) = \hat{\mathbf{D}}^H(\rho^{MA}) \quad (23)$$

The pseudocode in Algorithm 2 describes the process of constructing a Kriging surrogate model for predicting the effective elastic properties of graded microstructures, which reduces the computational cost of calculating effective properties by generating training samples and training the model to meet engineering precision requirements.

**Algorithm 2.** Construct a Kriging Surrogate Model for Predicting Effective Elastic Properties

---

**Input:**  $M, \rho, n, \rho_{\min}, \rho_{\max}$

// Step 1: Generate training sample set

```

1  for m=1 to M do
2      Uniformly sample density values  $\rho$  ranged from  $\rho_{\min}$  to  $\rho_{\max}$ ;
3      for  $\rho_e$  in Samples do
4          Call Algorithm.1 to obtain the corresponding shape interpolation coefficients;
5          Generate the level-set function of the graded microstructures in Eq. (13);
6          Compute effective elastic tensor  $\mathbf{D}$  via the homogenization method in Eqs.(15)-(16);
7          Add  $(\rho_e, \mathbf{D})$  to samples;
8      end for
9  end for
```

// Step 2: Train the Kriging model

```

10 Define the Kriging model via Eq.(17);
11 Estimate regression coefficients  $\boldsymbol{\beta}$  via Eq.(19);
12 Optimize hyperparameters by maximizing likelihood  $\boldsymbol{\theta}$  via Eq.(21);
// Step 3: Verify model convergence to meet engineering precision
```

```

13 if ModelAccuracy  $\geq \varepsilon$  then
14     break;
15 end if
16 iter = iter + 1;
17 if iter  $\geq \varepsilon$  then
18     break;
19 end if
20 n = n + 10;
21 goto Step 1
22 end while
```

---

**Output:** Trained Kriging surrogate model

---

Noted that  $m$  and  $n$  in Algorithm 1 represent the total number of the prototype microstructures and training samples obtained via uniform sampling, respectively, and  $\varepsilon$  denotes the accuracy tolerance. To qualitatively evaluate the prediction accuracy of the Kriging model, the relative error metric is defined as follows:

$$e_{rel} = \frac{\|\tilde{\mathbf{D}}^H - \mathbf{D}_{ref}^H\|_2}{\|\mathbf{D}_{ref}^H\|_2} \times 100\% \quad (24)$$

where  $\mathbf{D}_{ref}^H$  denotes reference effective properties via numerical homogenization, and  $\tilde{\mathbf{D}}^H$  denotes the predicted properties obtained from the Kriging model. Additionally, a test database consisting of randomly sampled points is generated for independent validation. The Root Mean Square Error (RMSE), is monitored for both the training set and the test set. The accuracy of the Kriging prediction model generally improves with an increasing number of training samples. The convergence study is typically conducted to determine the minimum sample size required to achieve user-defined precision, which is detailed in Section 5.1.

### 3.3. Multiscale topology optimization formulation for minimizing compliance

This section presents an efficient multi-scale topology optimization method based on spatially varying non-uniform microstructures. At the microscopic scale, the PLSM is employed to optimize multiple prototype microstructural configurations, which represent all non-uniform microstructures. At the macroscale, the Variable Thickness Sheet (VTS) method is employed to optimize the macroscopic material distribution. The proposed framework enables simultaneous optimization of the microstructural geometry and macroscopic distribution of the spatial-varying infills at a relatively low computational cost, yielding high-performance non-uniform porous structures.

It should be noted that the proposed framework is not a fully concurrent multiscale optimization. Instead, the Kriging surrogate model is pre-trained to map microstructure density to effective properties, and only the macroscale density is updated during optimization. This workflow is therefore termed surrogate-assisted multiscale topology optimization.

#### 3.3.1. Macroscopic structural optimization model

The objective function is to minimize the structural compliance subject to a given volume fraction. The topology optimization model based on the VTS method is formulated as follows:

$$\begin{aligned} \text{Find : } \rho^{MA} &= (\rho_1^{MA}, \rho_2^{MA}, \dots, \rho_{Ne}^{MA}), (Ne = 1, 2, \dots, NE) \\ \text{Min : } J &= \frac{1}{2} \int_{\Omega^{MA}} \varepsilon_{ij}^{(m)} \mathbf{D}_{ijkl}^{(m)} \varepsilon_{kl}^{(m)} d\Omega^{MA} + \frac{1}{2} \int_{\Omega} \varepsilon_{ij}^{(b)} \mathbf{D}_{ijkl}^{(b)} \varepsilon_{kl}^{(b)} d\Omega^{MA} \\ \text{S.t. } G(\rho^{MA}) &= \int_{\Omega^{MA}} \rho^{MA} V_0^{MA} d\Omega^{MA} - V^{MA} \leq 0 \\ a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \rho^{MA}) &= l(\mathbf{v}^{MA}), \forall \mathbf{v}^{MA} \in \bar{\mathbf{U}}(\Omega^{MA}) \\ \rho_{\min} &\leq \rho^{MA} \leq \rho_{\max} \end{aligned} \quad (25)$$

Where  $\rho_{Ne}^{MA}$  is the relative density of the  $Ne$ -th macroscopic finite element,  $\mathbf{v}^{MA}$  is the macroscopic virtual displacement field within the kinematically admissible displacement space  $\bar{\mathbf{U}}(\mathbf{u}^{MA})$ ,  $V_0^{MA}$  is the volume fraction of a solid element, and  $V^{MA}$  is the maximum allowable volume fraction for the macroscopic structure. The weak form of the elastic equilibrium condition is given by  $a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \rho^{MA}) = l(\mathbf{v}^{MA})$ , where the energy bilinear form  $a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \rho^{MA})$  and the load linear form  $l(\mathbf{v}^{MA})$  can be expressed as:

$$a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \rho^{MA}) = \int_{\Omega^{MA}} \varepsilon_{ij}(\mathbf{u}^{MA}) \mathbf{D}_{ijkl}^{MA}(\rho_{Ne}^{MA}) \varepsilon_{kl}(\mathbf{v}^{MA}) d\Omega^{MA} \quad (26)$$

$$l(\mathbf{v}^{MA}) = \int_{\Omega^{MA}} f \mathbf{v}^{MA} d\Omega^{MA} + \int_{\Gamma^{MA}} \tau \mathbf{v}^{MA} d\Gamma^{MA} \quad (27)$$

where  $f$  is the body force within the macroscopic domain,  $\tau$  is the traction force applied on the structural boundary  $\Gamma^{MA}$ .  $\mathbf{D}_{ijkl}^{MA}(\rho_{Ne}^{MA})$  is the elastic tensor of an equivalent density  $\rho_{Ne}^{MA}$ , which is obtained through an interpolation scheme as follows:

$$\mathbf{D}_{ijkl}^{MA}(\rho_{Ne}^{MA}) = \rho_{Ne}^{MA} \cdot (\mathbf{D}_{Ne}^0)_{ijkl} \quad (28)$$

where  $\mathbf{D}_{Ne}^0$  is the equivalent solid material property of the  $Ne$ -th macroscopic element. Each macroscopic element is treated as an individual microstructure, and thus the elastic tensor  $\mathbf{D}_{ijkl}^{MA}(\rho_{Ne}^{MA})$  of the  $Ne$ -th macroscopic element is equivalent to the elastic tensor  $\mathbf{D}_{ijkl}^H(\rho_{Ne}^{MA})$  of the microstructure with the same equivalent density. Therefore, it holds that:

$$(\mathbf{D}_{Ne}^0)_{ijkl} = \mathbf{D}_{ijkl}^H(\rho_{Ne}^{MA}) / \rho_{Ne}^{MA} \quad (29)$$

#### 3.3.2. Microscopic structural optimization model

Based on the PLSM with the compactly supported radial basis functions (CSRBFs) [54], the graded infill optimization aims to minimize structural compliance of elastic shell structures under a volume fraction constraint, which is formulated as:

$$\begin{aligned} \text{Find : } \alpha_{m,n} &(m = 1, 2, \dots, M; n = 1, 2, \dots, N) \\ \text{Min : } J &= \frac{1}{2} \int_{\Omega^{MA}} \varepsilon_{ij}^{(m)} \mathbf{D}_{ijkl}^{(m)} \varepsilon_{kl}^{(m)} d\Omega^{MA} + \frac{1}{2} \int_{\Omega} \varepsilon_{ij}^{(b)} \mathbf{D}_{ijkl}^{(b)} \varepsilon_{kl}^{(b)} d\Omega^{MA} \\ \text{S.t. } G_m(\alpha) &= \int_{\Omega_m} H(\Phi_m(\alpha)) d\Omega_m - \rho_m V_0 \leq 0 \\ a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \mathbf{D}_{ijkl}^H) &= l(\mathbf{v}^{MA}), \forall \mathbf{v}^{MA} \in \bar{\mathbf{U}}(\mathbf{u}^{MA}), \\ \tilde{\alpha}_{\min} &\leq \tilde{\alpha}_{m,n} \leq \tilde{\alpha}_{\max} \end{aligned} \quad (30)$$

The energy bilinear form can be further expressed as:

$$a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \mathbf{D}_{ijkl}^H) = \int_{\Omega^{MA}} \varepsilon_{ij}(\mathbf{u}^{MA}) \mathbf{D}_{ijkl}^H \varepsilon_{kl}(\mathbf{v}^{MA}) d\Omega^{MA} \quad (31)$$

where  $N$  is the number of nodes in the microscopic level-set discretization of a prototype microstructure,  $\alpha_{m,n}$  is the expansion coefficient of the CSRBF interpolation at the  $n$ -th node, which serves as the design variable.  $\mathbf{u}^{MA}$  is the macroscopic displacement field.  $\mathbf{v}^{MA}$  is the macroscopic virtual displacement field within the kinematically admissible displacement space  $\bar{\mathbf{U}}(\mathbf{u}^{MA})$ .  $V_0$  is the volume fraction. The normalized design variables are given by  $\tilde{\alpha}_{m,n}$ , with upper and lower bounds  $\tilde{\alpha}_{\min} = 0.001$  and  $\tilde{\alpha}_{\max} = 1$ , respectively.  $\Phi_m$  is the level-set function defined in the design domain of the  $m$ -th prototype microstructure, which is given by:

$$\Phi_m(\mathbf{x}, t) = \varphi_m(\mathbf{x}) \alpha_m(t) = \sum_{i=1}^N \varphi_{m,i}(\mathbf{x}) \cdot \alpha_{m,i}(t) \quad (32)$$

where  $\varphi_m(\mathbf{x})$  is the CSRBFs vector,  $t$  is an artificial pseudo-time to enable the dynamic motion of the shape deformations.

### 3.4. Sensitivity analysis and design variables update

In this work, a well-established and efficient Optimality Criteria (OC) [55–57] method is employed to update design variables. Thus, sensitivity analysis of the PLSM-based prototype microstructure optimization model is required.

#### 3.4.1. Sensitivity analysis and design variables update at macroscale

Based on the shape derivative [44], the sensitivity of the compliance

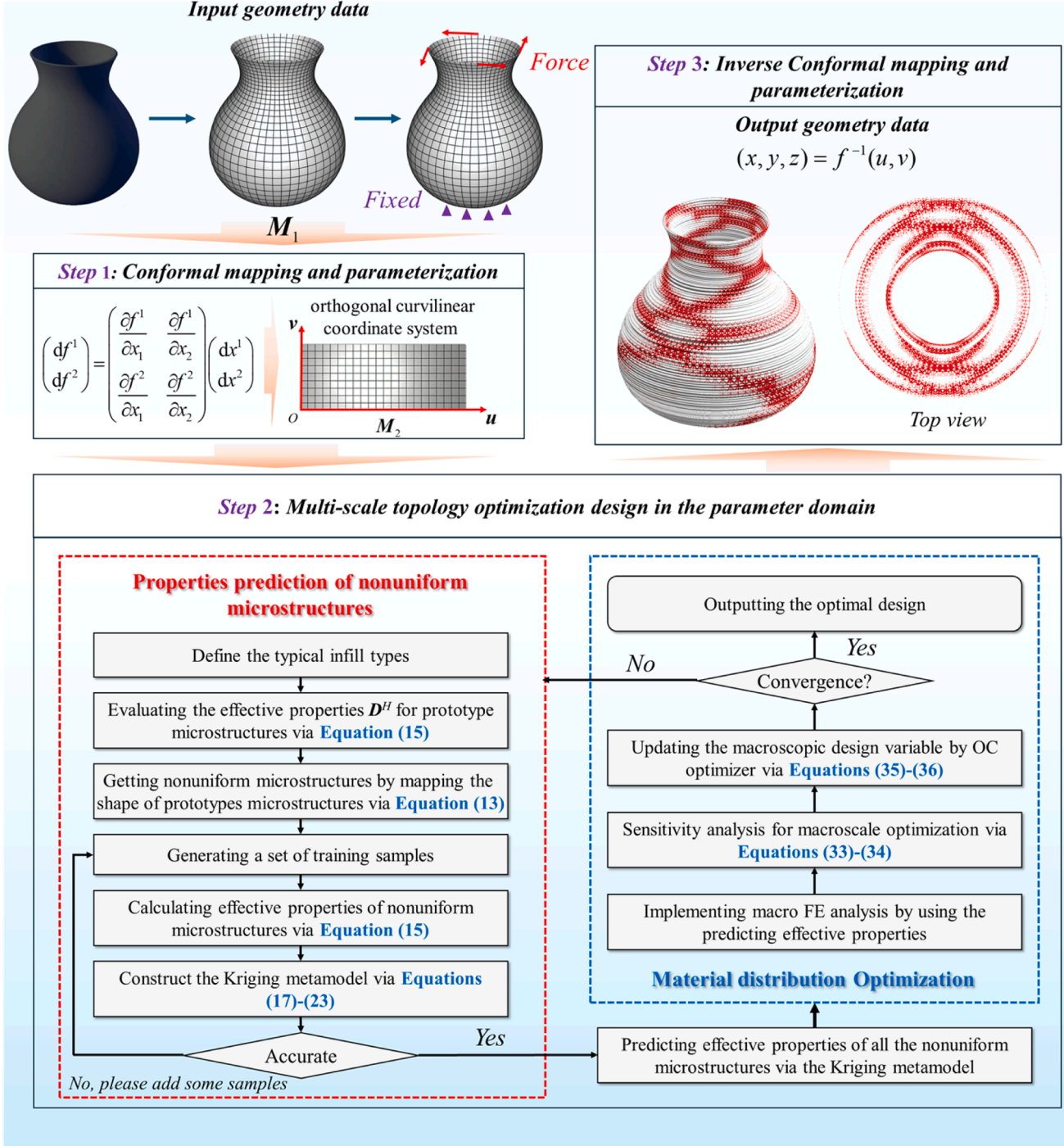


Fig. 6. Flowchart of the proposed graded infill optimization method.

$J$  with respect to the macroscopic design variable  $\rho_{Ne}^{MA}$  is derived as:

$$\frac{\partial J(\rho_{Ne}^{MA})}{\partial \rho_{Ne}^{MA}} = -\frac{1}{2} \left( \int_{\Omega_{Ne}^{MA}} \epsilon_{ij}^{(m)} (\mathbf{D}_{Ne}^{0(m)} (\rho_{Ne}^{MA})) \epsilon_{kl}^{(m)} d\Omega_{Ne}^{MA} + \int_{\Omega_{Ne}^{MA}} \epsilon_{ij}^{(b)} (\mathbf{D}_{Ne}^{0(b)} (\rho_{Ne}^{MA})) \epsilon_{kl}^{(b)} d\Omega_{Ne}^{MA} \right) \quad (33)$$

The sensitivity of the global volume constraint  $G$  with respect to the macroscopic design variable  $\rho_{Ne}^{MA}$  is derived as:

$$\frac{\partial G(\rho_{Ne}^{MA})}{\partial \rho_{Ne}^{MA}} = V_0^{MA} \quad (34)$$

Based on the above sensitivity information, the macroscopic design variables are updated using the OC algorithm:

0.001 and an upper bound  $\tilde{\alpha}_{\max} = 1$ . The normalized design variables  $\tilde{\alpha}_{m,n}$  can be updated based on the following heuristic scheme:

$$\tilde{\alpha}_{m,n}^{(k+1)} = \begin{cases} \min[(\eta + 1)\tilde{\alpha}_{m,n}^{(k)}, \tilde{\alpha}_{\max}], & \text{if } \min[(\eta + 1)\tilde{\alpha}_{m,n}^{(k)}, \tilde{\alpha}_{\max}] \leq [B_{m,n}^{(k)}]^{\zeta_{MA}} \tilde{\alpha}_{m,n}^{(k)} \\ [B_{m,n}^{(k)}]^{\zeta_{MA}} \tilde{\alpha}_{m,n}^{(k)}, & \text{if } \left\{ \begin{array}{l} \max[(1 - \eta)\tilde{\alpha}_{m,n}^{(k)}, \tilde{\alpha}_{\min}] < [B_{m,n}^{(k)}]^{\zeta_{MA}} \tilde{\alpha}_{m,n}^{(k)} \\ [B_{m,n}^{(k)}]^{\zeta_{MA}} \tilde{\alpha}_{m,n}^{(k)} < \min[(\eta + 1)\tilde{\alpha}_{m,n}^{(k)}, \tilde{\alpha}_{\max}] \end{array} \right. \\ \max[(1 - \eta)\tilde{\alpha}_{m,n}^{(k)}, \tilde{\alpha}_{\min}], & \text{if } [B_{m,n}^{(k)}]^{\zeta_{MA}} \tilde{\alpha}_{m,n}^{(k)} \leq \max[(1 - \eta)\tilde{\alpha}_{m,n}^{(k)}, \tilde{\alpha}_{\min}] \end{cases} \quad (41)$$

where  $B_{m,n}^{(k)}$  is defined as:

$$B_{m,n}^{(k)} = -\frac{\partial J(\alpha)}{\partial \alpha_{m,n}} \bigg/ \max \left( \vartheta, \Lambda_m^{(k)} \frac{\partial G(\alpha)}{\partial \alpha_{m,n}} \right) \quad (42)$$

$$\rho_{Ne}^{MA(k+1)} = \begin{cases} \min[\rho_{Ne}^{MA(k)} + \eta^{MA}, 1], & \text{if } \min[\rho_{Ne}^{MA(k)} + \eta^{MA}, 1] \leq [B_{Ne}^{MA(k)}]^{\zeta_{MA}} \rho_{Ne}^{MA(k)} \\ [B_{Ne}^{MA(k)}]^{\zeta_{MA}} \rho_{Ne}^{MA(k)}, & \text{if } \left\{ \begin{array}{l} \max[\rho_{\min}, \rho_{Ne}^{MA(k)} - \eta^{MA}] < [B_{Ne}^{MA(k)}]^{\zeta_{MA}} \rho_{Ne}^{MA(k)} \\ [B_{Ne}^{MA(k)}]^{\zeta_{MA}} \rho_{Ne}^{MA(k)} < \min[\rho_{Ne}^{MA(k)} + \eta^{MA}, 1] \end{array} \right. \\ \max[\rho_{\min}, \rho_{Ne}^{MA(k)} - \eta^{MA}], & \text{if } [B_{Ne}^{MA(k)}]^{\zeta_{MA}} \rho_{Ne}^{MA(k)} \leq \max[\rho_{\min}, \rho_{Ne}^{MA(k)} - \eta^{MA}] \end{cases} \quad (35)$$

where  $k$  is the iteration index,  $\eta^{MA}$  is a move limit, and  $\zeta_{MA}$  is a damping factor for numerical stability, which is set as 0.5 in this paper to ensure the stability of the iterative process. According to the optimality conditions, the parameter  $B_{Ne}^{MA(k)}$  is defined as:

$$B_{Ne}^{MA(k)} = -\frac{\partial C(\rho_{Ne}^{MA})}{\partial \rho_{Ne}^{MA}} \bigg/ \max \left( \vartheta, \Lambda^{MA(k)} \frac{\partial G(\rho_{Ne}^{MA})}{\partial \rho_{Ne}^{MA}} \right) \quad (36)$$

where  $\vartheta$  is a small positive constant introduced to avoid division by zero.  $\Lambda^{MA}$  is the Lagrange multiplier to the macroscopic design variable update, which can be iteratively updated using the bisection method.

#### 3.4.2. Sensitivity analysis and design variables update at the microscale

Based on the shape derivative [44] and a series of derivations provided in Appendix B, the first-order derivative of the objective function with respect to the design variables can be obtained as follows:

$$\frac{\partial J(\alpha)}{\partial \alpha_{n,n}} = -\frac{1}{2} \left( \int_{\Omega^{MA}} \epsilon_{ij}^{(m)} \frac{\partial \mathbf{D}_{ijkl}^{H(m)}}{\partial \alpha_{n,n}} \epsilon_{kl}^{(m)} d\Omega^{MA} + \int_{\Omega^{MA}} \epsilon_{ij}^{(b)} \frac{\partial \mathbf{D}_{ijkl}^{H(b)}}{\partial \alpha_{n,n}} \epsilon_{kl}^{(b)} d\Omega^{MA} \right) \quad (37)$$

The derivative of the local volume constraint with respect to the design variables can be given by:

$$\frac{\partial G_m(\alpha)}{\partial \alpha_{m,n}} = \int_{\Omega_m} \varphi_{m,n}(x) \cdot \delta(\Phi_m) d\Omega_m \quad (38)$$

Due to the difficulty in determining the upper and lower bounds of the design variables during the optimization process, normalization of these variables is first performed to facilitate numerical implementation:

$$\tilde{\alpha}_{m,n}^{(k)} = \frac{\alpha_{m,n}^{(k)} - \alpha_{m,\min}^{(k)}}{\alpha_{m,\max}^{(k)} - \alpha_{m,\min}^{(k)}} \quad (39)$$

where

$$\alpha_{m,\min}^{(k)} = 2 \times \min(\alpha_{m,n}^{(k)}), \alpha_{m,\max}^{(k)} = 2 \times \max(\alpha_{m,n}^{(k)}) \quad (40)$$

The normalized design variables  $\tilde{\alpha}_{m,n}$  have a fixed lower bound  $\tilde{\alpha}_{\min} =$

Finally, the design variables  $\alpha_{m,n}^{(k+1)}$  are recovered from the updated normalized design variables  $\tilde{\alpha}_{m,n}^{(k+1)}$  as follows:

$$\alpha_{m,n}^{(k+1)} = \tilde{\alpha}_{m,n}^{(k+1)} \times (\alpha_{m,\max}^{(k)} - \alpha_{m,\min}^{(k)}) + \alpha_{m,\min}^{(k)} \quad (43)$$

#### 4. Numerical implementation and computing environment

The proposed optimization framework for graded infill design of thin-walled curved shell structures follows a three-stage Map-Design-Inverse workflow, as illustrated in Fig. 6. All numerical implementations are carried out in MATLAB R2024b on a standard personal computer equipped with an Intel Core i9 CPU (8 cores) and 32 GB of memory.

##### Stage 1: Conformal mapping and parameterization.

The design process begins by extracting the mid-surface of the target curved shell structure. Based on the conformal geometry theory, the free-form surface of the original shell structure is mapped onto a planar rectangular parameter domain through an angle-preserving transformation. The parameter domain is subsequently discretized into a structured and uniform mesh.

##### Stage 2: Multiscale topology optimization design in the parameter domain.

With the parameter domain established, the topology optimization of macroscopic material distribution and microscopic graded microstructures is performed. At the microscopic scale, a set of prototype microstructures is first defined using the parametric level-set functions. These prototypes are designed to be connectable by employing a shape interpolation scheme to generate a continuous family of graded microstructures. The corresponding interpolation coefficients are determined using a bisection algorithm that iteratively adjusts them until the effective density of the interpolated microstructure matches the target value within a specified tolerance. Then, a Kriging-based surrogate model is constructed to effectively predict the effective elastic tensor for any given microstructure density. The procedure involves the following steps:

Step 1: Generate a set of training samples by uniformly sampling density values within the feasible range [0.1, 0.9].



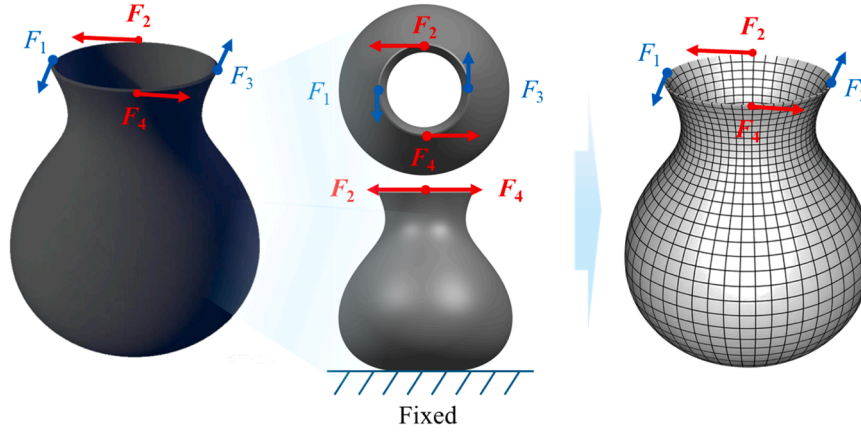


Fig. 7. The vase shell design domain and boundary conditions.

Step 2: For each sample density, compute the corresponding shape interpolation coefficient using Algorithm 1 and generate the level-set function of the graded microstructure via Eq. (13).

Step 3: Evaluate the effective elastic tensor  $\mathbf{D}$  via numerical homogenization by solving the microscale equilibrium equation on the periodic unit cell, as described in Eqs. (15)–(16).

Step 4: Train a Kriging model using Algorithm 2 that maps the input density  $\rho$  to the predicted effective properties  $\tilde{\mathbf{D}}^H(\rho)$  via Eq. (17).

Step 5: Evaluate the prediction accuracy using the relative error metric defined in Eq. (24) and compute the RMSE for both the training set and a separate validation set.

Step 6: If the accuracy criteria are not met, refine the training process using an adaptive sampling strategy. Specifically, identify regions of the density range where prediction errors are highest and add more training samples specifically in those regions. The refinement loop continues until the surrogate model achieves the required accuracy, after which it is deemed ready for integration into the optimization framework. If the accuracy criteria are satisfied, the trained Kriging model is used throughout the optimization process to provide instant predictions of effective properties for any given density, without further calls to the homogenization solver.

The graded infill optimization problem is then formulated to minimize the structural compliance. At each optimization iteration, the design variables at two scales are updated using the OC method based on the sensitivity information. Additionally, the optimization process is terminated if any of the following convergence criteria are met: (1) The relative changes in both the objective function  $|c^{(k)} - c^{(k-1)}|/c^{(k)}$  and the design variable vector  $||\varphi^{(k)} - \varphi^{(k-1)}||_\infty$  between consecutive iterations fall below a tolerance of  $10^{-3}$ ; (2) The metric quantifying the change or oscillation of the material interface (e.g., based on the change in the perimeter or the level-set field) is also reduced below  $10^{-3}$ , indicating a stable topological configuration; (3) A predefined maximum number of iterations 500 is reached as a safeguard against excessive computation.

#### Stage 3: Inverse conformal mapping.

Upon the convergence of the optimization in the parameter domain, the resulting graded infill configuration represented by the assembled global level-set function is mapped back onto the original curved shell surface via the inverse conformal transformation. This inverse mapping yields the final multi-scale thin-walled shell structures with optimized graded infill, where the solid, boundary, and void regions are clearly defined.

## 5. Numerical examples

In this section, two numerical examples are presented to validate the proposed conformal mapping-based graded infill optimization method for curved thin-walled structures, which integrates the Kriging surrogate

model for efficient property prediction. The first example uses a vase shell to demonstrate the conformal mapping and graded infill optimization on a curved surface with varying curvature. The second example employs a turbine blade shell to further establish the generality and engineering applicability of the proposed method to free-form surfaces.

For the convenience of discussion and comparison, all physical quantities presented herein are dimensionless. Young's modulus  $E = 1$  and Poisson's ratio  $\mu = 0.3$ . A uniform shell thickness of  $T = 1$  is adopted throughout the entire design domain.

### 5.1. Vase shell

The geometry of the vase shell is provided as an STL file, which can be downloaded from the repository link provided in Appendix C. As shown in Fig. 7, the bottom of the vase is fixed, and four tangential loads are applied on the top of the vase with magnitudes  $F_1 = F_3 = 0.1$  and  $F_2 = F_4 = 0.15$ . After a mesh sensitivity study, the vase shell is conformally mapped to a regular 2D plane and discretized into structured meshes consisting of  $48 \times 80$  four-node plane elements. Consequently, the vase surface is discretized into 3840 conformal shell elements after conformal mapping, each filled with a graded microstructure. The global volume fraction is set to 0.3.

#### 5.1.1. Property estimation of graded infill microstructures

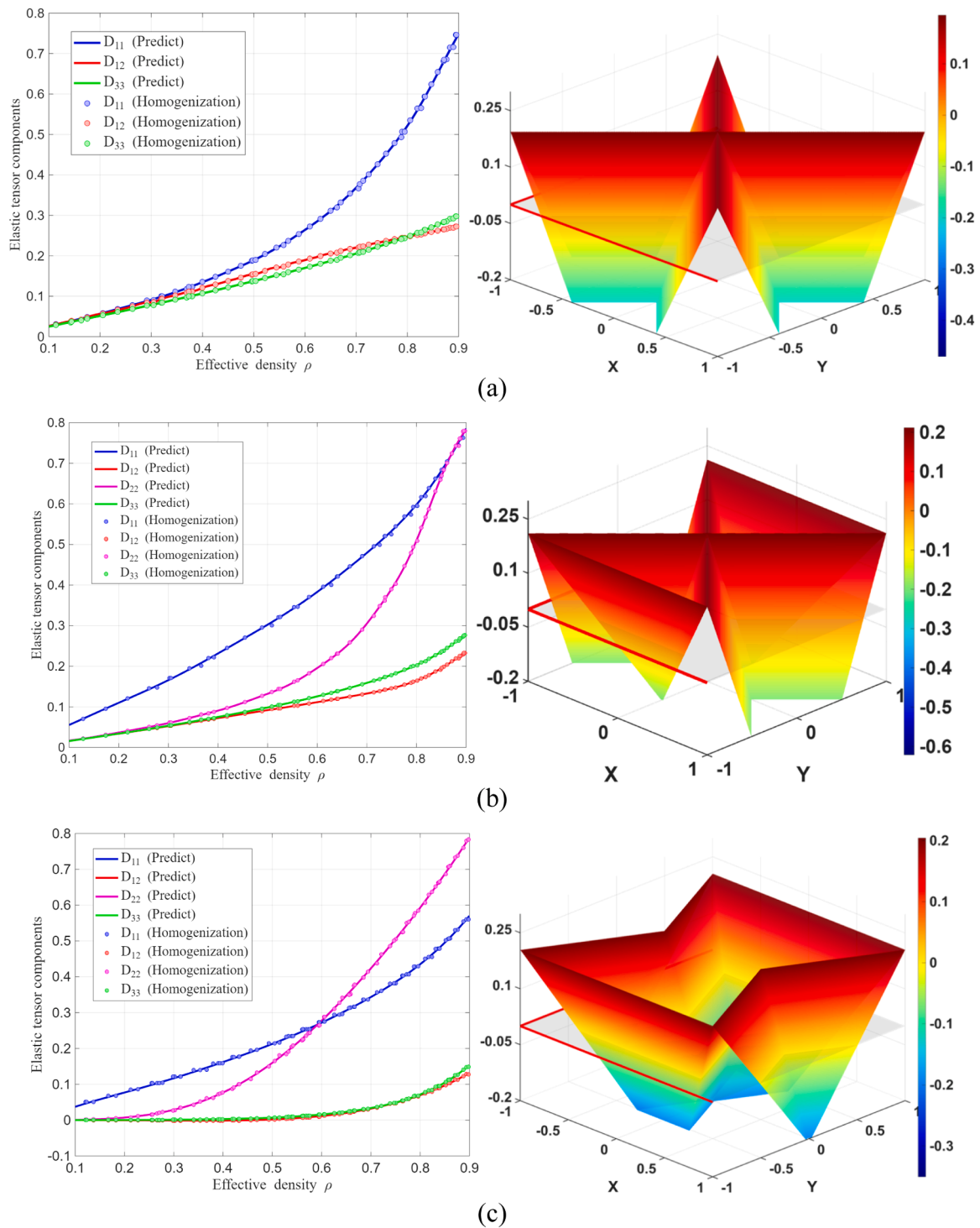
Given the orthotropic symmetry of the graded infill microstructures, the equivalent elasticity coefficient matrices can be expressed as:

$$\mathbf{D}_{mic} = \begin{bmatrix} D_{11} & D_{12} & 0 \\ D_{21} & D_{22} & 0 \\ 0 & 0 & D_{33} \end{bmatrix} \quad (44)$$

where  $\mathbf{D}_{mic}$  generally contains nine effective property parameters. However, due to the orthogonal anisotropy of the infill microstructures, the off-diagonal components are symmetric such that  $D_{12} = D_{21}$ . This symmetry reduces the number of independent parameters to four effective property parameters  $D_{11}$ ,  $D_{12}$ ,  $D_{22}$ , and  $D_{33}$ , where  $D_{11}$  and  $D_{22}$  represent the effective stiffnesses along the two orthogonal principal directions,  $D_{12}$  represents the Poisson coupling effect between these directions, and  $D_{33}$  denotes the effective shear stiffness. They provide a complete description of the effective mechanical response of the orthotropic graded infill structures employed in this work.

There is a special case: for X-shaped microstructures, the geometric symmetry further implies  $D_{11} = D_{22}$ .

To evaluate the predictive performance of the Kriging-based surrogate model for different infill microstructures, we uniformly sampled 50 density points from the range  $[0.1, 0.9]$  as the training set, as shown in Fig. 8, and randomly selected an additional 30 density points as the test set. For the X-shaped infill, the RMSE on the training set is only 0.0347%



**Fig. 8.** Property estimation of three different graded infill microstructures. (a) Fill type 1: X-shaped microstructures, (b) Fill type 2: eight-shaped microstructures, (c) Fill type 3: Concave hexagon-shaped microstructures.

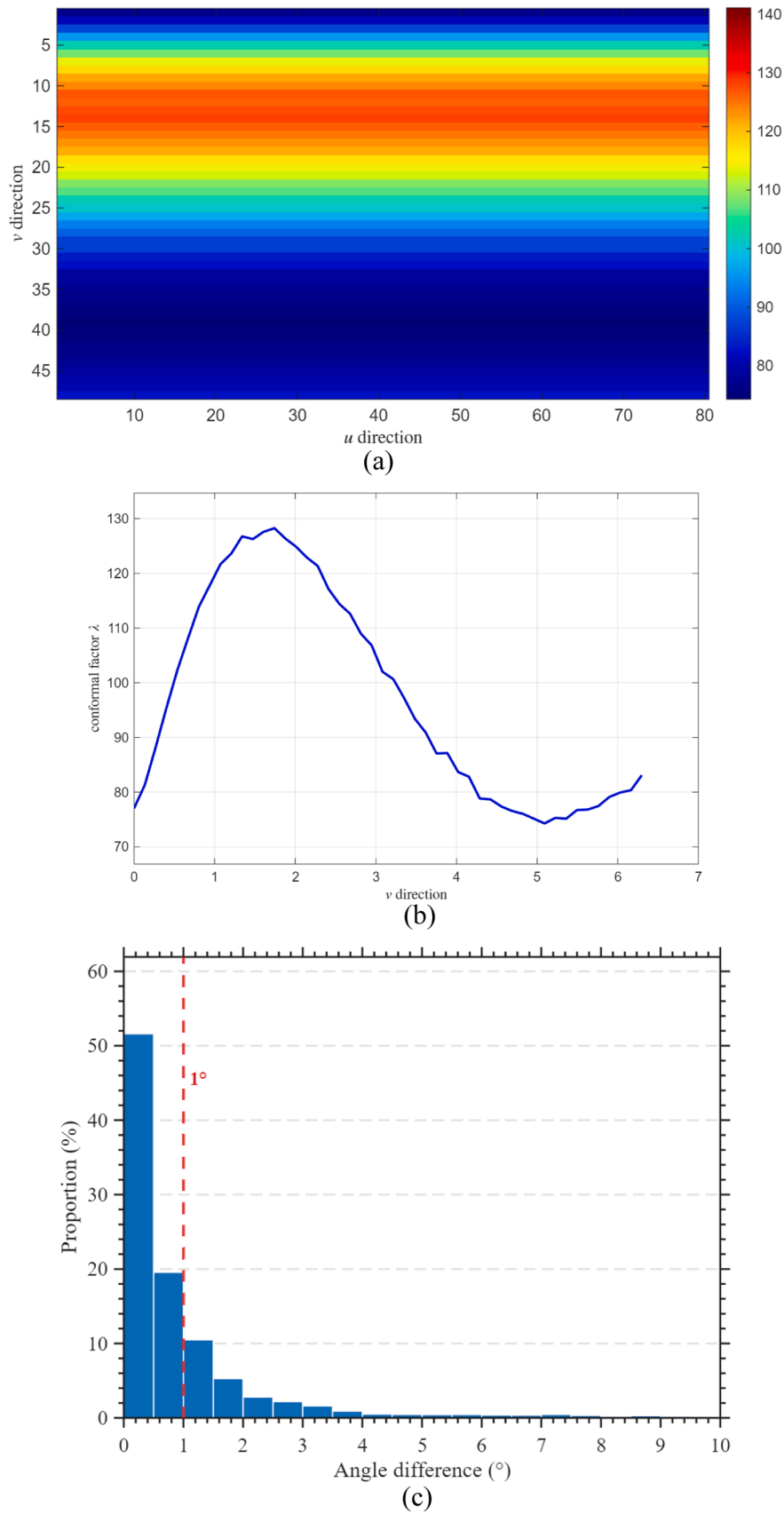
while the RMSE on the test set is 0.202%. For the eight-shaped infill type, the RMSE on the training set is 0.0370% while the RMSE on the test set is 0.314%. For the concave hexagon-shaped infill type. The RMSE on the training set is only 0.0634% while the RMSE on the test set is 0.276%. These results demonstrate that the surrogate model achieves excellent training accuracy across all three microstructure types.

Remarkably, Zhang et al. [44] demonstrated that for the multiscale design of a 2D L-shaped beam, only 10 microstructure samples per prototype were required to construct a Kriging model with

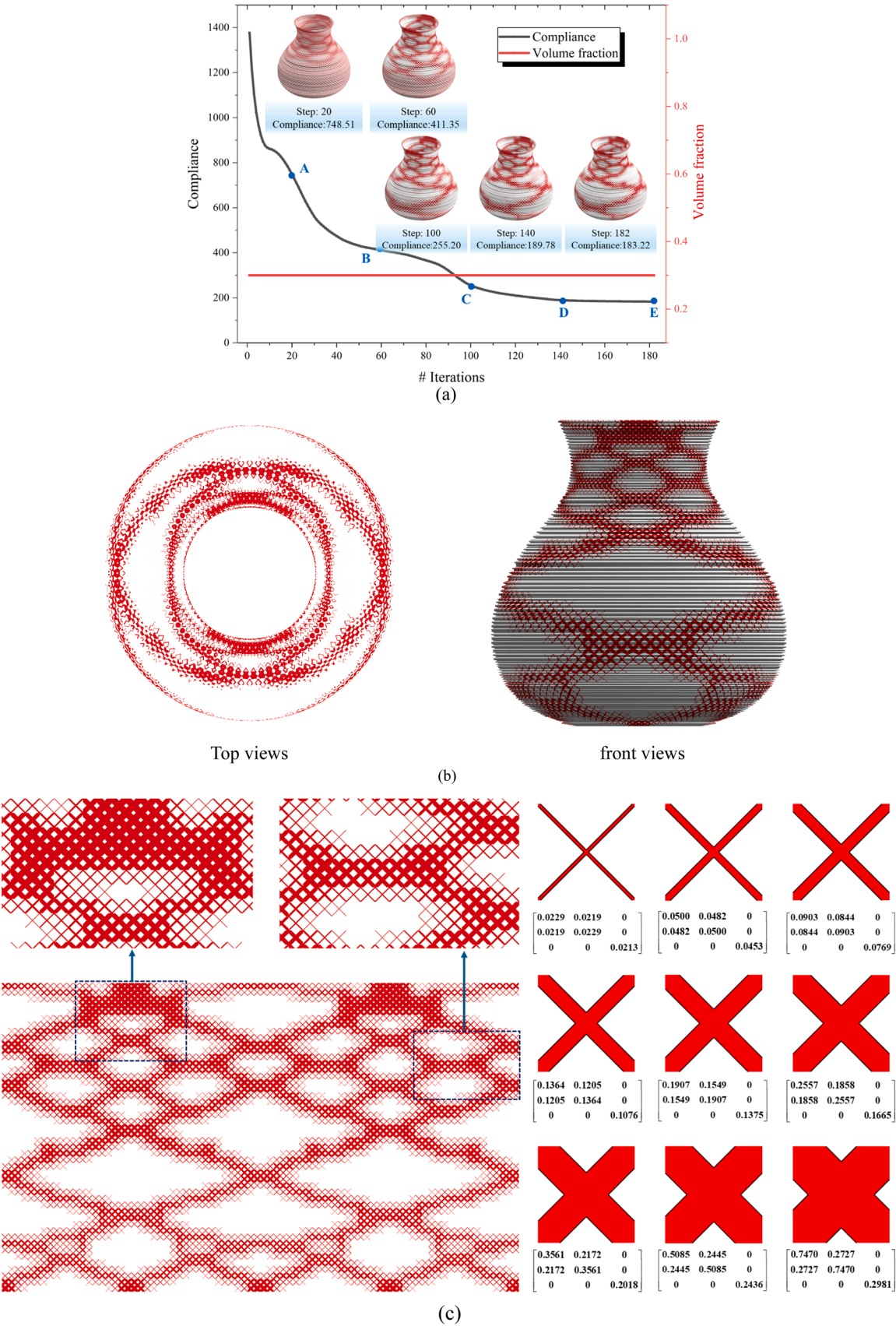
engineering-acceptable prediction accuracy. In our study, the use of a larger training dataset further enhances the predictive reliability of the proposed data-driven approach for graded infill design.

Prior to the optimization, the conformal mapping from the 3D vase shell surface to the 2D rectangular parametric domain is performed. To quantitatively characterize the resulting area distortion, the distribution of the conformal factor  $\lambda(u,v)$  is computed across all macroscopic elements and is illustrated in Fig. 9.

For the vase shell example, the conformal factor ranges from  $\lambda_{\min}$

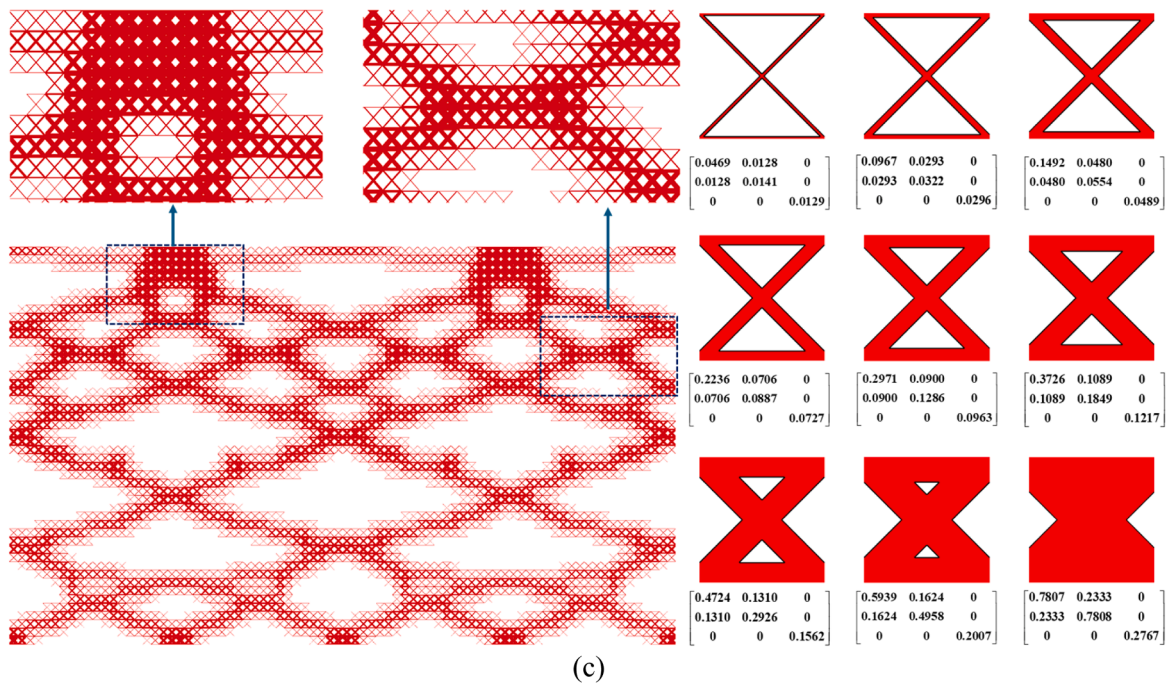
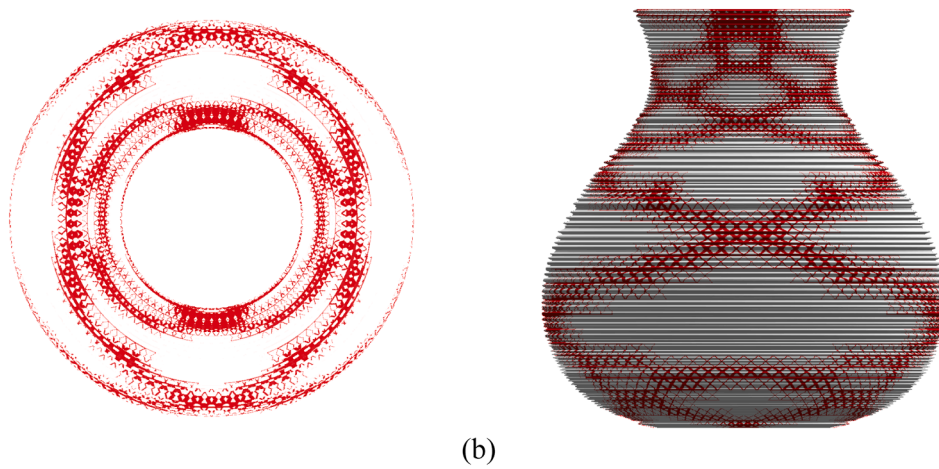
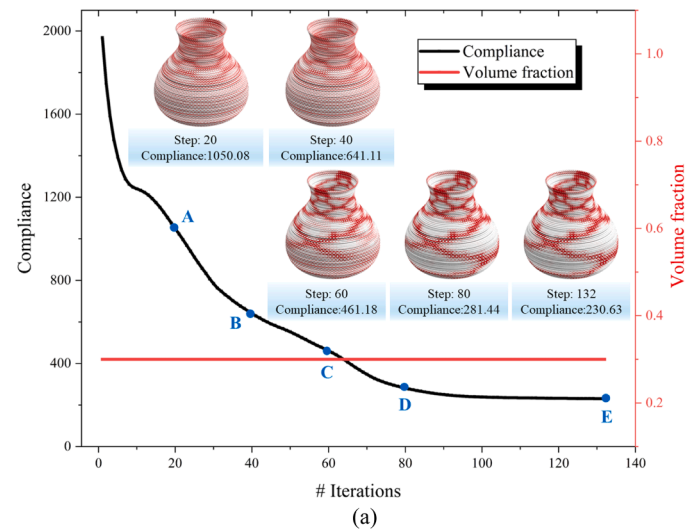


**Fig. 9.** Conformal mapping distortion analysis. (a) Distribution of the conformal factor  $\lambda(u, v)$  over the 2D parametric domain of the vase shell. Regions with larger  $\lambda$  correspond to areas of higher local curvature on the original 3D surface, (b) Variation of conformal factor along v direction, (c) Angle distortion of the conformal mapping.

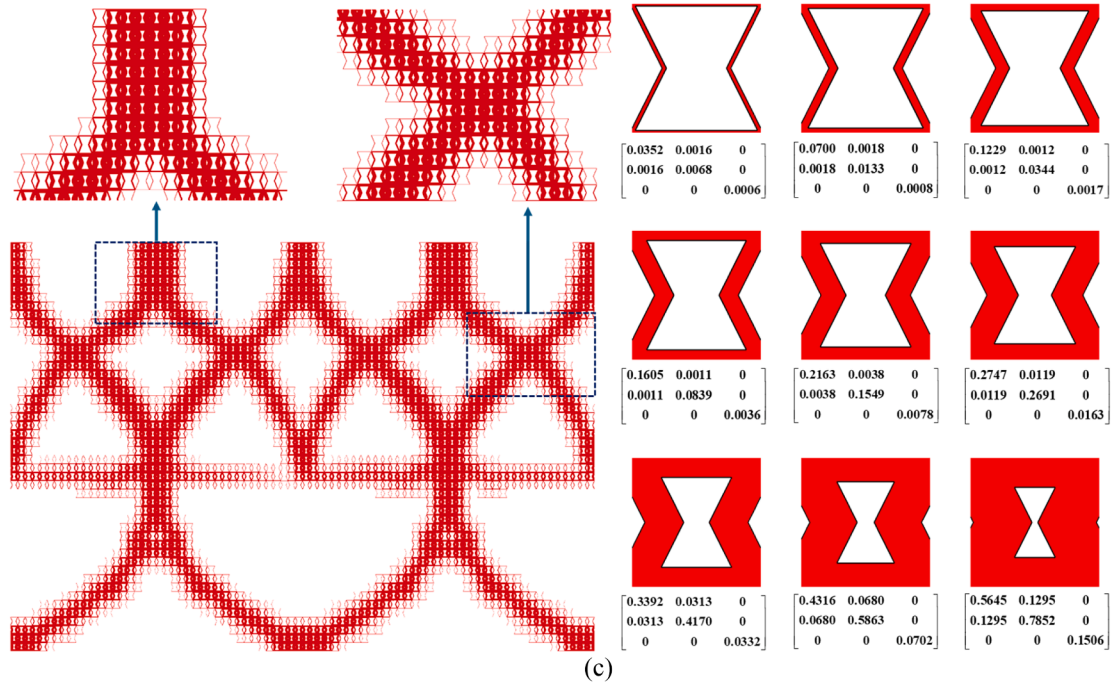
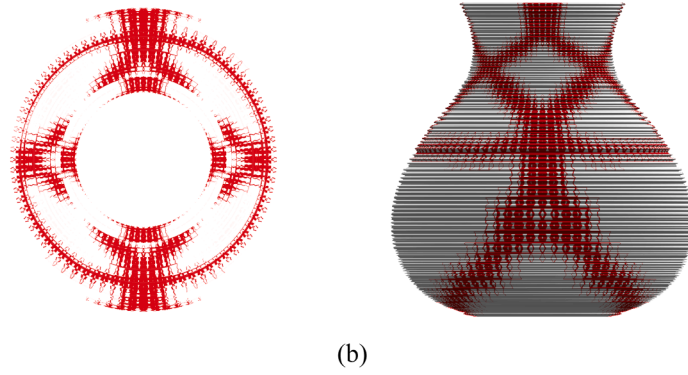
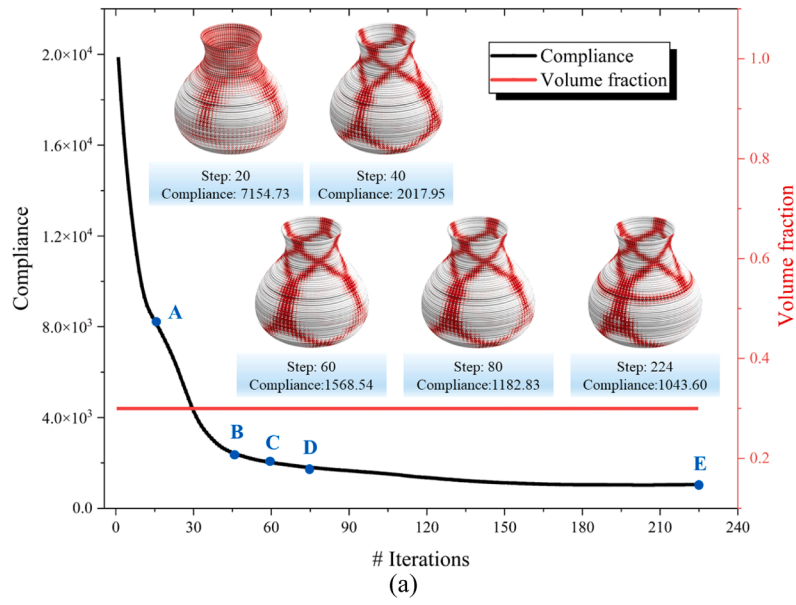


**Fig. 10.** Graded infill design optimization results for the vase shell with X-shaped infill microstructures. (a) Iterative convergence history of compliance, volume fraction, and topological configuration for the vase shell with X-shaped microstructures, (b) Top and front views of the optimized topological configuration for the vase shell with X-shaped microstructures, (c) Conformal mapping onto a 2D rectangular parametric domain, and several parametric microstructures with graded properties are listed with the following equivalent elasticity coefficient.





**Fig. 11.** Graded infill design optimization results for the vase shell with eight-shaped infill microstructures. (a) Iterative convergence history of compliance, volume, and topological configuration for the vase shell with eight-shaped microstructures, (b) Top and front views of the optimized topological configuration for the vase shell with eight-shaped microstructures, (c) Conformal mapping onto a 2D rectangular parametric domain, and several parametric microstructures with graded properties are listed with the following equivalent elasticity coefficient.



**Fig. 12.** Graded infill design optimization results for the vase shell with concave hexagon-shaped infill microstructures. (a) Iterative convergence history of compliance, volume, and topological configuration for the vase shell with concave hexagon-shaped microstructures, (b) Top and front views of the optimized topological configuration for the vase shell with concave hexagon-shaped microstructures, (c) Conformal mapping onto a 2D rectangular parametric domain, and several parametric microstructures with graded properties are listed with the following equivalent elasticity coefficient.

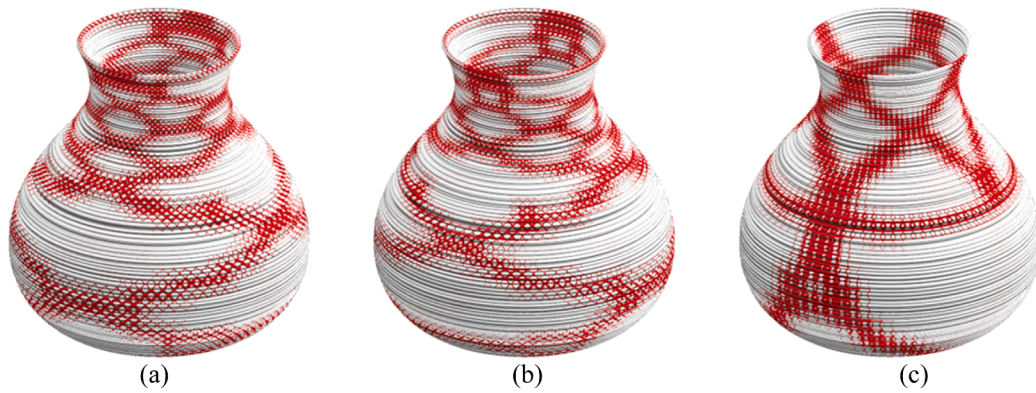


Fig. 13. Comparison of optimized vase shell designs formed by three infill types: (a) X-shaped, (b) Eight-shaped, and (c) Concave hexagon-shaped microstructures.

$= 74.28$  to  $\lambda_{\max} = 128.08$ , The distortion ratio  $\lambda_{\max}/\lambda_{\min} = 1.72$  indicates that the linear scale factor varies by a factor of approximately 1.72 across the shell surface. In terms of element area, the actual 3D area of the largest element is approximately 2.96 times that of the smallest element, reflecting the variation in local curvature across the vase geometry. The distortion is most pronounced near the neck of the vase, where the local curvature is highest. At the same time, the angle differences are predominantly concentrated in the low-distortion region, with the majority being within  $1^\circ$ . This confirms that the conformal mapping preserves angles with acceptable fidelity for the vase shell geometry considered in this study.

Despite this area distortion, the conformal shell finite element formulation rigorously accounts for it through the Lamé coefficients: the actual 3D area of each element is computed as  $\lambda^2 \cdot du \cdot dv$ , and all stiffness integrations are performed with respect to the actual physical area rather than the uniform parametric area. Consequently, the macroscale structural response is correctly evaluated. Moreover, since conformal mapping acts as a locally isotropic scaling, the topology and orientation of each microstructure are preserved during the inverse mapping, with no directional distortion introduced.

#### 5.1.2. Multiscale topology optimization result under different infill types

To investigate the influence of different infill microstructures on the overall structural performance of the vase shell, three types of microstructures were employed as the infill pattern, including X-shaped, eight-shaped, and concave hexagon-shaped microstructures. Each microstructure exhibits distinct topological characteristics and mechanical properties, enabling a comprehensive comparison of their effectiveness in multi-scale topology optimization. The optimization results for the vase shell with different infill microstructures are shown in Figs. 10–12.

The convergence histories for the vase shell with three infill types are illustrated in Figs. 10–12 (a), respectively. In all cases, the compliance decreases rapidly within the first 50 iterations, accompanied by

significant redistribution of the graded microstructures. Beyond this stage, the objective function curves become relatively flat and stable, indicating successful convergence to the optimal topological configuration. Among the three infill types, the optimized designs exhibit distinct differences, primarily attributed to the varying elastic properties of the unit cell for each configuration, as shown in Fig. 13. This variation consequently influences the distribution of the graded microstructures. Furthermore, the compliance values for the optimized vase shell corresponding to the three infill types are 183.22, 230.63, and 1043.60, respectively. At an equivalent global volume fraction, the optimized design with X-shaped microstructures yields the lowest compliance.

Figs. 10–12 (b) show the top and front views of the optimized topological configurations for the vase shell with three infill types, respectively. Due to the central symmetry of the applied loads and the underlying assumption of linear elasticity, both the intermediate steps and the final optimized results exhibit axisymmetric and centrosymmetric characteristics. During the iteration steps, the distribution pathways of high-density microstructures gradually become more distinct, aligning primarily with the structure's main load-transfer paths. All microstructures remain fully conformal to the shell surface. In addition, as observed from the locally enlarged views of the optimized results, the graded microstructures are interconnected due to their geometrically similar configurations. Under the prescribed global volume constraint, the optimized graded infill shell achieves a rational distribution of microstructures with varying volume fractions, thereby effectively improving the overall structural stiffness.

To facilitate the visualization and characterization of the graded microstructures, the optimized density distributions over the 2D rectangular parametric domain prior to inverse conformal mapping are presented in Figs. 10–12 (c). Several representative graded microstructures with densities ranging from 0.1 to 0.9 are extracted and displayed together with their corresponding equivalent elastic coefficients. These coefficients quantitatively characterize the gradual variation in mechanical properties across the shell surface for each infill pattern.

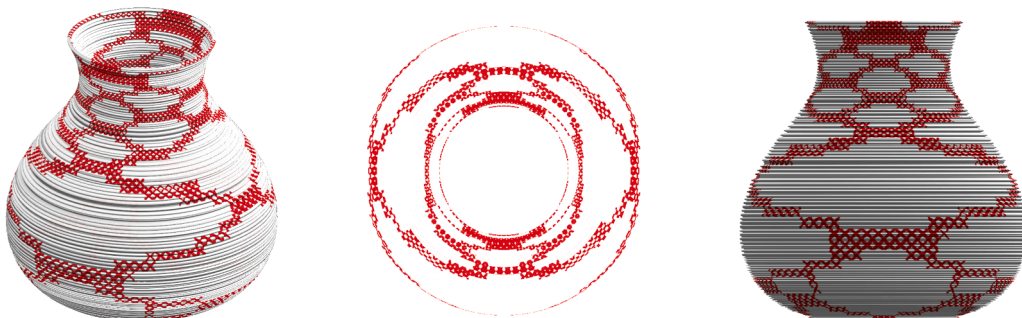
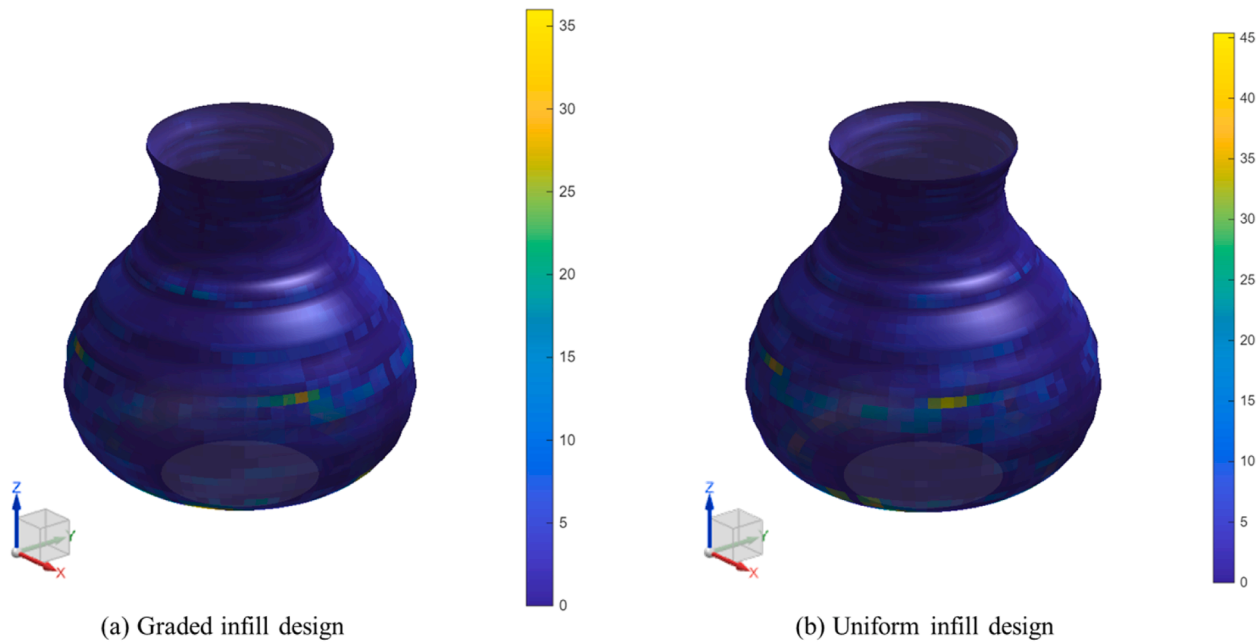


Fig. 14. Optimization results of the vase shell with X-shaped microstructures at a global volume fraction of 0.3.





**Fig. 15.** Comparison of displacement distributions of the vase shell with X-shaped microstructures: (a) graded infill design with a maximum displacement of 35.65; (b) uniform infill design with a maximum displacement of 45.39.

#### 5.1.3. Comparison with existing methods

To benchmark the performance of the proposed method, the optimization result of the vase shell with X-shaped microstructures is compared with several reference designs under the same global volume fraction of 0.3. The optimized graded infill design of the vase shell with X-shaped microstructures yields a compliance of 183.33, whereas the uniform infill design with the same global volume fraction achieves a compliance of 266.65, as shown in Fig. 14. Compared with the uniform design, the optimized design achieves a 31.25% reduction in compliance. As observed from the displacement distribution illustrated in Fig. 15, the graded design leads to a significant reduction in the structural deformation relative to the uniform design. Specifically, the maximum displacement of the graded infill design is 35.65, while that of the uniform design reaches 45.39, corresponding to a reduction of

approximately 21.46%. This improvement arises because multi-scale optimization effectively broadens the design space, enabling a more efficient load transfer mechanism and significantly enhancing the deformation resistance of the multiscale curved-shell structure.

Furthermore, without considering microscale graded infill, the conventional single-scale topology optimization using the SIMP method on the flattened parametric domain results in a compliance of 198.45, which is 8.3% higher than the proposed multi-scale result. This comparison demonstrates that the topology optimization of macro-scale material distribution and micro-scale graded infill configurations leads to superior structural performance by enabling more efficient load transfer through tailored local stiffness.

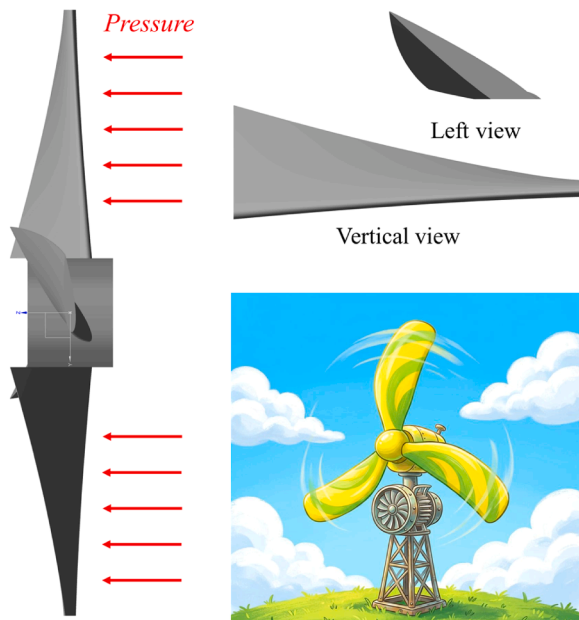
It should be noted that for surfaces with extremely high curvature or for applications requiring ultra-high precision, the curvature-induced distortion may not be negligible. A more rigorous approach would involve solving the homogenization problem directly on the curved unit cell. Nevertheless, for the vase shell structure considered in this work, the curvature is relatively moderate.

#### 5.1.4. Computational efficiency analysis

The computational cost of the proposed framework is analyzed to demonstrate its efficiency. The vase shell example with 3840 macroscopic elements was optimized using three different strategies: (1) the proposed Kriging-assisted method, (2) conventional multiscale optimization with on-the-fly homogenization at each iteration, and (3) direct 3D optimization without dimensionality reduction.

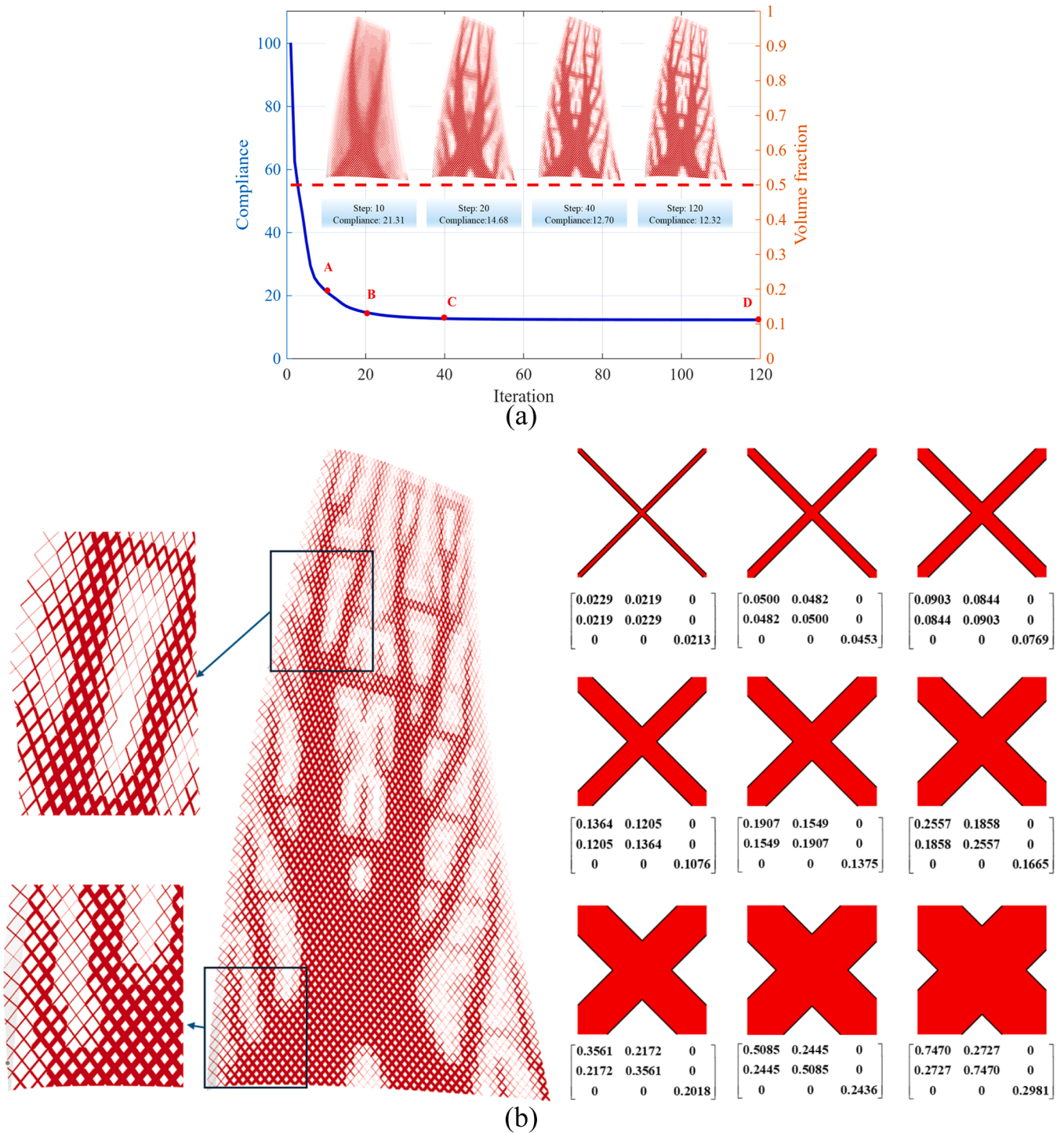
The conventional method requires approximately 8.2 min per iteration, primarily due to repeated finite element homogenization for each microstructure candidate. In contrast, the proposed Kriging-assisted method reduces this to approximately 0.67 min per iteration, achieving a speedup factor of approximately 12.24 per iteration. For the main optimization loop, the total computational time of the proposed method is approximately 4.5 h, compared to 41.0 h for the conventional method, confirming an approximately  $9 \times$  overall speedup. The offline Kriging training requires an additional 3.2 h with 50 training samples per prototype, a one-time cost that is negligible when the same microstructure family is reused.

In terms of memory usage, the peak memory consumption of the proposed framework is approximately 1.2 GB, well within the capacity



**Fig. 16.** The design domain and boundary conditions of the turbine blade shell.





**Fig. 17.** Graded infill design optimization results for the blade shell with X-shaped infill microstructures. (a) Iterative convergence history of compliance, volume fraction, and topological configuration for the blade shell with X-shaped microstructures, (b) Several parametric microstructures with graded properties are listed with the following equivalent elasticity coefficient.

of a standard workstation with 32 GB RAM. The dominant memory cost arises from the global stiffness matrix of the macroscale shell FEM, which scales linearly with the number of degrees of freedom.

However, direct 3D optimization of the curved shell with the same resolution is computationally infeasible, requiring an estimated ten thousand elements and exceeding 48 h for a single iteration. These results confirm that the combination of conformal mapping and Kriging surrogate modeling makes the multi-scale optimization of curved thin-

walled structures computationally tractable.

## 5.2. Turbine blade shell

To demonstrate the engineering applicability of the proposed framework on a free-form surface, a second example involving a turbine blade is presented. Turbine blades are critical load-bearing components in aero-engines and gas turbines, characterized by complex, doubly-

curved free-form surfaces with spanwise twist and chordwise camber. Their lightweight design under aerodynamic loading is of direct relevance to engine efficiency and thrust-to-weight ratio. In contrast to the closed, axisymmetric vane shell, the turbine blade is a non-axisymmetric free-form surface subjected to a distributed aerodynamic pressure and constrained at the root, thereby providing a test of the generality and robustness of the proposed framework.

As individual blades in a turbomachinery assembly are subjected to identical loading and can be designed independently owing to the cyclic symmetry of the rotor, the optimization of a single blade is representative of the entire blade row, as shown in Fig. 16. The blade geometry features spanwise variation in chord length, twist angle, and sweep, yielding a representative free-form blade surface. The blade is modeled as a hollow shell structure. The MATLAB code used to generate the STL file of the blade shell is provided in Appendix D.

The blade root is fully constrained to represent its connection to the rotor disk. A distributed aerodynamic load of up to 1.5 kPa is applied to the blade surface, with higher intensity near the leading edge. The free-form surface is discretized into 2400 conformal shell elements. The X-shaped microstructure is adopted as the infill prototype, and the Kriging surrogate model trained in Section 5.1 is directly reused. The global volume fraction is set to 0.5.

The optimization results the turbine blade shell are presented in Fig. 17. The proposed framework converges after 120 iterations, yielding a final compliance of 12.32. The optimized graded infill distribution exhibits higher-density microstructures concentrated near the blade root and along the principal load paths, where the structural response to the aerodynamic pressure is most significant. This example confirms that the proposed framework is applicable to free-form engineering structures, thereby establishing its generality and robustness.

## 6. Conclusions and future work

This paper presents a conformal mapping-based multiscale topology optimization framework for the design of graded infill microstructures in thin-walled curved shells, addressing the critical challenges of high computational cost and geometric fidelity in lightweight shell component design. The main contributions and findings of this work are summarized as follows:

- (1) The Map-Design-Inverse workflow based on conformal mapping effectively reduces the dimensionality of graded infill design on 3D curved surfaces. By conformally mapping the original free-form shell surface onto a 2D parametric domain, the complexity associated with direct 3D optimization is substantially reduced. Moreover, the angle-preserving property of conformal mapping guarantees geometric fidelity when the optimized infill is mapped back to the original surface, thereby bridging the gap between design simplicity and geometric complexity.
- (2) The prototype microstructures are defined using a parameterized level-set method, and a continuous family of graded microstructures is generated via the shape interpolation scheme. It ensures topological similarity and connectivity between adjacent microstructures. The effective elastic tensor is computed using numerical homogenization, and a Kriging-based surrogate model is developed to predict the effective mechanical properties of graded microstructures with high accuracy. Numerical results show that the root mean square error on the test set is below 0.32% for three distinct infill types, including X-shaped, eight-shaped, and concave hexagon-shaped microstructures. This surrogate model replaces the computationally expensive numerical homogenization during optimization iterations, significantly reducing computational cost while maintaining prediction reliability.
- (3) The vane shell example demonstrates that the optimized graded infill design achieves a 31.25% reduction in compliance and a

21.46% reduction in maximum displacement compared with a uniform infill design under the same global volume fraction, confirming the effectiveness of the proposed framework in enhancing structural stiffness. Among the three infill types investigated, the X-shaped configuration yields the lowest compliance of 183.22, attributable to its superior elastic properties. This result indicates that the topological characteristics of microstructures significantly influence the overall performance of thin-walled shell structures, providing valuable guidance for infill pattern selection in engineering applications. In addition, the turbine blade example converges to an optimized design with a final compliance of 12.32, confirming the applicability of the method to free-form engineering surfaces.

Future work will focus on three main directions: (1) incorporating geometric nonlinearity and large deformation capabilities to address highly flexible shell structures; (2) developing adaptive or online learning strategies for surrogate model updates, reducing or eliminating the need for pre-training; (3) introducing smooth density-gradient constraints, higher-order homogenization, or multiscale stress analysis to more rigorously address local stress concentration and the limitations of the periodic homogenization assumption in regions with strong density variations between adjacent cells.

## Replication of results

The results presented in this paper can be replicated using software Matlab. The data and codes will be available once requested.

## Author contribution

The authors' contributions are as follows: Jian Wang was responsible for the conceptualization, methodology, formal analysis, data curation, software, and original draft writing. Qiang Gao was responsible for the supervision and conceptualization. Liuchao Jin was responsible for the methodology and draft writing. Wei-Hsin Liao was responsible for the investigation, review, editing, project administration, and funding acquisition.

## CRediT authorship contribution statement

**Jian Wang:** Writing – original draft, Software, Methodology, Formal analysis, Data curation, Conceptualization. **Wei-Hsin Liao:** Writing – review & editing, Project administration, Investigation, Funding acquisition. **Qiang Gao:** Supervision, Conceptualization. **Liuchao Jin:** Writing – original draft, Methodology.

## Ethical approval

This study does not involve human participants, animal subjects, or ethical concerns requiring institutional approval.

## Declaration of Competing Interest

The authors claim that the paper is based on very recently completed original research, and has neither been published elsewhere nor been submitted for publication to any other journal. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Appendix A. Nomenclature

| Symbol                           | Description                                          |
|----------------------------------|------------------------------------------------------|
| $ds_i$                           | Infinitesimal arc elements on surface $M_i$          |
| $r_i(x^1, x^2)$                  | Local coordinate system on surface $M_i$             |
| $f$                              | Conformal mapping                                    |
| $\lambda(x^1, x^2)$              | Conformal factor                                     |
| $\mathbf{x}$                     | Spatial coordinates                                  |
| $(u, v)$                         | Orthogonal curvilinear coordinate system             |
| $\varepsilon_{uv}$               | Normal strains                                       |
| $\varepsilon_{uv}$               | Shear strain                                         |
| $\tau$                           | Distance from one point to the mid-surface           |
| $\chi_{uv}$                      | Changes in principal curvature                       |
| $\chi_{uv}$                      | Twist rate                                           |
| $A, B$                           | Lamé coefficients                                    |
| $E$                              | Young's modulus                                      |
| $\mu$                            | Poisson's ratio                                      |
| $T$                              | Thickness of the conformal shell                     |
| $D$                              | Constitutive matrix                                  |
| $\Omega$                         | Set of all admissible shapes                         |
| $\Phi$                           | Level set function                                   |
| $\partial\Omega$                 | Structural boundary                                  |
| $\varphi_e$                      | Shape interpolation coefficient                      |
| $ne$                             | Total number of microstructures                      |
| $\rho$                           | Relative density                                     |
| $f_{pm}$                         | Lower bound of relative density                      |
| $\mathbf{v}$                     | Virtual displacement field                           |
| $\bar{\mathbf{U}}(\Omega_{m,e})$ | Kinematically admissible periodic displacement field |
| $\beta$                          | Vector of regression coefficients                    |
| $\hat{\beta}$                    | Generalized least square estimator                   |
| $Z(\rho^{MA})$                   | Gaussian random process                              |
| $\mathbf{R}$                     | Correlation matrix                                   |
| $\theta$                         | Hyper-parameter                                      |
| $L(\theta)$                      | Likelihood function                                  |
| $\mathbf{D}_{ref}^H$             | Reference effective property                         |
| $\bar{\mathbf{D}}^H$             | Predicted effective property                         |
| $t$                              | Artificial pseudo-time                               |
| $V$                              | Volume fraction                                      |
| $\alpha$                         | Expansion coefficient                                |
| $\bar{\alpha}$                   | Normalized design variable                           |
| $\varphi_m(x)$                   | Compactly supported radial basis function            |
| $J$                              | Objective function (compliance)                      |
| $G$                              | Volume constraint                                    |
| $k$                              | Iteration index                                      |
| $\eta$                           | Move limit                                           |
| $\varsigma$                      | Damping factor                                       |
| $\varepsilon$                    | Tolerance                                            |
| $e_{rel}$                        | Relative error                                       |
| $m$                              | Total number of the prototype microstructures        |
| $n$                              | Total number of training samples                     |

## Appendix B. Sensitivity analysis of the design variables

This section presents the detailed derivation of the sensitivity with respect to the design variables, which are defined as the expansion coefficients of the compactly supported radial basis function interpolation used in the optimization of prototype microstructures.

The shape derivatives of the objective function  $J(\alpha)$ , state equation  $(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \mathbf{D}_{ijkl}^H)$  and  $l(\mathbf{v}^{MA})$  can be respectively given by:

$$\frac{\partial J(\alpha)}{\partial t} = \frac{1}{2} \int_{\Omega^{MA}} \left[ 2\varepsilon_{ij}^{(m)} \mathbf{D}_{ijkl}^{H(m)} \varepsilon_{kl}^{(m)} + \varepsilon_{ij}^{(m)} \frac{\partial \mathbf{D}_{ijkl}^{H(m)}}{\partial t} \varepsilon_{kl}^{(m)} + 2\varepsilon_{ij}^{(b)} \mathbf{D}_{ijkl}^{H(b)} \varepsilon_{kl}^{(b)} + \varepsilon_{ij}^{(b)} \frac{\partial \mathbf{D}_{ijkl}^{H(b)}}{\partial t} \varepsilon_{kl}^{(b)} \right] d\Omega^{MA} \quad (B1)$$

$$\frac{\partial a}{\partial t} = \int_{\Omega^{MA}} \left[ 2\varepsilon_{ij}^{(m)} \mathbf{D}_{ijkl}^{H(m)} \varepsilon_{kl}^{(m)} + \varepsilon_{ij}^{(m)} \frac{\partial \mathbf{D}_{ijkl}^{H(m)}}{\partial t} \varepsilon_{kl}^{(m)} + 2\varepsilon_{ij}^{(b)} \mathbf{D}_{ijkl}^{H(b)} \varepsilon_{kl}^{(b)} + \varepsilon_{ij}^{(b)} \frac{\partial \mathbf{D}_{ijkl}^{H(b)}}{\partial t} \varepsilon_{kl}^{(b)} \right] d\Omega^{MA} \quad (B2)$$

$$\frac{\partial l}{\partial t} = \int_{\Omega^{MA}} f \mathbf{v}^{MA} d\Omega^{MA} + \int_{\Omega^{MA}} \tau \mathbf{v}^{MA} d\Gamma^{MA} \quad (B3)$$

To consider the term  $\mathbf{v}^{MA}$ , the adjoint equation is established as follows:

$$\int_{\Omega^{MA}} \varepsilon_{ij} \mathbf{D}_{ijkl}^H \varepsilon_{kl} d\Omega^{MA} = \int_{\Omega^{MA}} f \mathbf{v}^{MA} d\Omega^{MA} + \int_{\Omega^{MA}} \tau \mathbf{v}^{MA} d\Gamma^{MA} \quad (\text{B4})$$

The bilinear energy form for the macroscopic thin-shell structure is expressed as:

$$a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \mathbf{D}_{ijkl}^H) = \int_{\Omega^{MA}} \varepsilon_{ij}(\mathbf{u}^{MA}) \mathbf{D}_{ijkl}^H \varepsilon_{kl}(\mathbf{v}^{MA}) d\Omega^{MA} \quad (\text{B5})$$

Differentiating the above Eq. (B5) with respect to  $t$  yields:

$$\frac{\partial a(\mathbf{u}^{MA}, \mathbf{v}^{MA}, \mathbf{D}_{ijkl}^H)}{\partial t} = \frac{\partial l(\mathbf{v}^{MA})}{\partial t} \quad (\text{B6})$$

Substituting Eqs. (B2)-(B4) into Eq. (B5) yields:

$$\int_{\Omega^{MA}} \varepsilon_{ij} \mathbf{D}_{ijkl}^H \varepsilon_{kl} d\Omega^{MA} = - \int_{\Omega^{MA}} \varepsilon_{ij} \frac{\partial \mathbf{D}_{ijkl}^H}{\partial t} \varepsilon_{kl} d\Omega^{MA} \quad (\text{B7})$$

Considering that the compliance optimization is a self-adjoint problem, the shape derivative of the objective function can be rewritten by substituting Eq. (B7) into Eq. (B1) as follows:

$$\frac{\partial J(\alpha)}{\partial t} = -\frac{1}{2} \left( \int_{\Omega^{MA}} \varepsilon_{ij}^{(m)} \frac{\partial \mathbf{D}_{ijkl}^{H(m)}}{\partial t} \varepsilon_{kl}^{(m)} d\Omega^{MA} + \int_{\Omega^{MA}} \varepsilon_{ij}^{(b)} \frac{\partial \mathbf{D}_{ijkl}^{H(b)}}{\partial t} \varepsilon_{kl}^{(b)} d\Omega^{MA} \right) \quad (\text{B8})$$

The derivative of  $\mathbf{D}_{ijkl}^H$  with respect to  $t$  is given by:

$$\frac{\partial \mathbf{D}_{ijkl}^H}{\partial t} = \frac{1}{|\Omega_m|} \int_{\Omega_m} \left( \varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^* \right) \mathbf{D}(\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^*) v_m \cdot |\nabla \Phi_m| \delta(\Phi_m) d\Omega_m \quad (\text{B9})$$

where  $\delta(\Phi_m) = \frac{1}{\pi} \frac{\xi}{(\Phi_m)^2 + \xi^2}$  is the derivative of the Heaviside function  $H(\Phi_m)$ , and  $\xi$  is a small positive value typically chosen as two to four times the element size,  $v_m$  is the normal velocity, which is denoted as follows:

$$v_m = \frac{\varphi_m(\mathbf{x})}{|\nabla \varphi_m(\mathbf{x}) \alpha_m(t)|} \frac{d\alpha_m(t)}{dt} \quad (\text{B10})$$

Substituting Eq. (B10) into Eq. (B9), we can get the following equation:

$$\frac{\partial \mathbf{D}_{ijkl}^H}{\partial t} = \sum_{n=1}^N \left( \frac{1}{|\Omega_m|} \int_{\Omega_m} \left( \varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^* \right) \mathbf{D}(\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^*) \varphi_{m,n}(\mathbf{x}) \cdot \delta(\Phi_m) d\Omega_m \right) \cdot \frac{\partial \alpha_{m,n}}{\partial t} \quad (\text{B11})$$

Then, applying the chain rule, the derivative of  $\mathbf{D}_{ijkl}^H$  with respect to  $t$  can also be given by:

$$\frac{\partial \mathbf{D}_{ijkl}^H}{\partial t} = \sum_{n=1}^N \frac{\partial \mathbf{D}_{ijkl}^H}{\partial \alpha_{m,n}} \cdot \frac{\partial \alpha_{m,n}}{\partial t} \quad (\text{B12})$$

Thus, the derivative of  $\mathbf{D}_{ijkl}^H$  with respect to the design variables  $\alpha_{m,n}^{MI}$  can be expressed as:

$$\frac{\partial \mathbf{D}_{ijkl}^H}{\partial \alpha_{m,n}^{MI}} = \frac{1}{|\Omega_m|} \int_{\Omega_m} \left( \varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^* \right) \mathbf{D}(\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^*) \varphi_{m,n}^{MI}(\mathbf{x}) \cdot \delta(\Phi_m) d\Omega_m \quad (\text{B13})$$

Recalling Eq. (B12) and substituting Eq. (B3) into Eq. (B12) yields:

$$\frac{\partial J(\alpha)}{\partial t} = -\frac{1}{2} \sum_{m=1}^M \left( \int_{\Omega^{MA}} \varepsilon_{ij}^{(m)} \left[ \sum_{n=1}^N \frac{\partial \mathbf{D}_{ijkl}^{H(m)}}{\partial \alpha_{m,n}^{MI}} \cdot \frac{\partial \alpha_{m,n}^{MI}}{\partial t} \right] \varepsilon_{kl}^{(m)} d\Omega^{MA} + \int_{\Omega^{MA}} \varepsilon_{ij}^{(b)} \left[ \sum_{n=1}^N \frac{\partial \mathbf{D}_{ijkl}^{H(b)}}{\partial \alpha_{m,n}^{MI}} \cdot \frac{\partial \alpha_{m,n}^{MI}}{\partial t} \right] \varepsilon_{kl}^{(b)} d\Omega^{MA} \right) \quad (\text{B14})$$

The derivative of the objective function with respect to  $t$  can be given by:

$$\frac{\partial J(\alpha)}{\partial t} = \sum_{m=1}^M \sum_{n=1}^N \frac{\partial J(\alpha)}{\partial \alpha_{m,n}} \frac{\partial \alpha_{m,n}}{\partial t} \quad (\text{B15})$$

Comparing the corresponding terms in Eqs. (B14) and (B15), the final sensitivity of the objective function  $J(\alpha)$  with respect to  $\alpha_{m,n}$  can be obtained as:

$$\frac{\partial J(\alpha)}{\partial \alpha_{m,n}} = -\frac{1}{2} \left( \int_{\Omega^{MA}} \varepsilon_{ij}^{(m)} \frac{\partial \mathbf{D}_{ijkl}^{H(m)}}{\partial \alpha_{m,n}} \varepsilon_{kl}^{(m)} d\Omega^{MA} + \int_{\Omega^{MA}} \varepsilon_{ij}^{(b)} \frac{\partial \mathbf{D}_{ijkl}^{H(b)}}{\partial \alpha_{m,n}} \varepsilon_{kl}^{(b)} d\Omega^{MA} \right) \quad (\text{B16})$$

This completes the sensitivity derivation, which enables gradient-based optimization of the prototype microstructures using the Optimality Criteria



(OC) method.

## Appendix C. Vase shell

Please download the Supplementary materials Appendix C.zip.

## Appendix D. The MATLAB code for the geometry generation of turbine blade shell

---

```
function generate_blade_stl(filename)
% Parameters of Turbine blade
span = 2.0; % Span length
nz = 70; % Spanwise segments
nc = 60; % Chordwise segments
chord0 = 1.0; % Root chord length
chordT = 0.6; % Tip chord length
twist0 = 25; % Root twist angle
twistT = -10; % Tip twist angle
thick = 0.12; % Relative thickness
% Upper and lower surfaces
beta = linspace(0, pi, nc);
xc = 0.5*(1 - cos(beta));
yt = 5*thick*(0.2969*sqrt(xc) - 0.1260*xc - 0.3516*xc.^2 ...
+ 0.2843*xc.^3 - 0.1015*xc.^4);
xprof = [xc, fliplr(xc)];
yprof = [yt, -fliplr(yt)];
npc = length(xprof);
V = zeros(nz*npc, 3);
for k = 1:nz
s = (k-1)/(nz-1);
chord = chord0 + (chordT-chord0)*s;
tw = (twist0 + (twistT-twist0)*s) * pi/180;
% Section scaling
xp = (xprof - 0.25) * chord;
yp = yprof * chord;
% Spanwise twist
xr = xp*cos(tw) - yp*sin(tw);
yr = xp*sin(tw) + yp*cos(tw);
sweep = 0.15*s^2;
zpos = span*s;
V((k-1)*npc + (1:npc),:) = [xr(:) + sweep, yr(:), zpos*ones(npc,1)];
end
% Triangular facets
F = [];
for k = 1:nz-1
for m = 1:npc
mp = mod(m, npc) + 1;
a = (k-1)*npc + m; b = (k-1)*npc + mp;
c = k*npc + mp; d = k*npc + m;
F = [F; a b c; a c d];
end
end
% Write binary STL file
fid = fopen(filename, 'w');
fwrite(fid, zeros(80,1,'uint8'), 'uint8');
fwrite(fid, size(F,1), 'uint32');
for t = 1:size(F,1)
p = V(F(t,:),:);
n = cross(p(2,:)-p(1,:), p(3,:)-p(1,:));
n = n / (norm(n) + 1e-30);
fwrite(fid, single([n, p(1,:), p(2,:), p(3,:)]), 'float32');
fwrite(fid, 0, 'uint16');
end
fclose(fid);
end
```

---

## Data availability

Data will be made available on request.

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