

Topology optimization of coated structures
considering multiple scales, multiple materials,
and non-uniform coating thickness

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KYOTO UNIVERSITY

DOCTORAL THESIS

**Topology Optimization of Coated Structures Considering Multiple
Scales, Multiple Materials, and Non-uniform Coating Thickness**

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of the

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February 25, 2025

Declaration of Authorship

I, Tiannan Hu, declare that this thesis titled, “Topology Optimization of Coated Structures Considering Multiple Scales, Multiple Materials, and Non-uniform Coating Thickness” and the work presented in it are my own. I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
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- I have acknowledged all main sources of help.
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Signed:

Date:

关山难越 谁悲失路之人

兴尽悲来 识盈虚之有数

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KYOTO UNIVERSITY

Abstract

Strength of Materials and Structures Lab
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Doctor of Philosophy

Topology Optimization of Coated Structures Considering Multiple Scales, Multiple Materials, and Non-uniform Coating Thickness

by Tiannan Hu

This thesis focuses on the optimum design of multiscale and multimaterial coated structures using topology optimization (TO) technique. A novel concurrent multiscale TO framework to design coated structures with layer-wise lattice infill microstructures is firstly developed with the maximization of the fundamental eigenfrequency, in which structures at two scales are simultaneously optimized. To deal with multiple eigenfrequencies, the modal assurance criteria (MAC) method is introduced and its effectiveness is proved. Then, this new multiscale TO framework is extended to minimum dynamic compliance design by optimizing coated structures infilled with layer-wise bi-material lattice microstructures under time-harmonic excitation frequency. Specially, a new mathematical model with a static compliance constraint is constructed, which ensures the success of structural optimization under an excitation frequency higher than the fundamental eigenfrequency. Motivated by the popular trend of designing multi-material structures, a new TO method for the optimum design of coated structures infilled with multiple materials is also developed, where a novel material interpolation model for the topology description is proposed based on the ordered solid isotropic material with penalization (SIMP) scheme. The coating, the substrate, and the material distribution of the multi-material infilling can be well identified using several modified design variables via smoothing and projection techniques. This density-based filtering procedure for designing coated structures is then extended to multiscale problem by specifying different optimized microstructures for varied macroscale material blocks. To ensure the microstructural connectivity, the designable connective region (DCR) method is introduced, and thus coated structures infilled with multiple self-connected microstructures are achieved. In addition, the non-uniform coating of coated structures is optimized via a newly developed density-based TO approach to realize better structural performance, and body-fitted mesh is implemented for smooth structural boundaries.

Keywords: Multiscale topology optimization, coated structures, multi-material design, velocity field-based level-set method, ordered SIMP method, fundamental eigenfrequency, dynamic compliance, non-uniform coating thickness

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Dedicated to my mother and my grandparents

To my sincere friends

Chapter 1

General Introduction

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1.1 Introduction

Undergone rapid development over decades of years, structural optimization has been widely applied in industries such as aerospace, marine engineering, and architecture. Generally, it can be divided into three categories, i.e., size optimization, shape optimization, and topology optimization. Size optimization, firstly proposed by O. Schmit in 1960 (Schmit, 1960), focuses on optimizing the dimensions of structural members (such as the cross-sectional areas) while adhering to given constraints, just as its name indicates. The introduction of size optimization marked a major milestone, laying the foundation for computational optimization techniques and serving as a cornerstone of modern structural optimization. Using size optimization, designers can improve structural performance by adjusting several specific CAD parameters, however, the improvement is limited due to the maintenance of shape or topology and no innovative structural form can be generated. Shape optimization, introduced by Gallagher and Zienkiewicz in 1970s (Gallagher and Zienkiewicz, 1973), involves modifying the dimensions and shape of structures by optimizing their moving boundaries. Compared to size optimization, it is more effective in enhancing structural performance. However, it does not allow changes to the structural topology, which limits the design flexibility and the extent of optimization achievable. Overcoming the shortcomings of size optimization and shape optimization, topology optimization (TO) provides enhanced design flexibility which enables the simultaneous optimization of structures' size,

shape, and topology, effectively identifying the optimal material distribution within the design domain and maximizing the potential of materials. Therefore, TO is widely regarded as the most powerful mathematical design tool and has attracted the attention of numerous scholars and engineers. Since the pioneering research made by Bendsoe and Kikuchi in 1988 (Bendsøe and Kikuchi, 1988), TO has been utilized in a variety of problems, including stiffener layout optimization to enhance load-carrying capacity (Li, Qu, Luo, and Liu, 2021; Zhang, Ding, Wang, Ni, and Li, 2020; Li, Gao, Zhou, Chen, Yin, and Zhang, 2023), acoustic material design for noise isolation (Yoon, 2013; Kim and Yoon, 2015; Lu, Yamamoto, Otomori, Yamada, Izui, and Nishiwaki, 2013), heat exchanger design that maximizes the heat transfer efficiency (Saviers, Ranjan, and Mahmoudi, 2019; Fawaz, Hua, Le Corre, Fan, and Luo, 2022), bone implant optimization for facial reconstruction (Sutradhar, Paulino, Miller, and Nguyen, 2010; Zegard and Paulino, 2016; Xiong, Ding, Zhang, Hu, Xu, Duan, and Huang, 2024), and so on. Building upon the achievements of predecessors, this thesis aims to propose novel TO methods for designing bio-inspired coated structures that take into account multiple scales and materials.

The reminder of this chapter is organized as follows: In Section 1.2, we provide a brief review of several typical TO methods, i.e., density method, evolutionary method, and level set method. Section 1.3 briefly describes the sensitivity analysis using the basic stiffness optimization formulations, with three approaches to sensitivity calculation are discussed, i.e., finite difference method, direct difference method, as adjoint method, along with a detailed derivation of the shape sensitivity. The motivation behind this thesis is illustrated in Section 1.4. Eventually, the overall structure of this thesis is outlined in Section 1.5.

1.2 Shape and topology optimization methods

In this section, we introduce the brief concept of several TO methods with their merits and demerits. Three popular TO methods are selected as examples to understand the key points of optimum design using the TO technique, including density method, evolutionary method, and level set methods. It should be noted that there are plenty of other TO approaches, such as bionic design methods (adaptive growth method (Hu, Ding, Shen, and Zhang, 2020) and leaf-vein bifurcation method (Li, Hong, Yan, and Liu, 2013)) and the feature driven methods (method of moving morphable components (Zhang, Li, Yuan, Song, and Guo, 2017) and method of moving morphable voids (Du, Yao, Zhao, and Chen, 2019)). Due to space limitation and research interests, they will not be elaborated upon in this thesis.

1.2.1 Density method

The most widely used TO method in both academia and industry is definitely the density method (Sigmund, 2001; Tarek and Ray, 2020). This approach introduces the concept of pseudo-density for each discretized element of the design domain to represent the presence or absence of material. Two typical schemes can be integrated with the density design variable ρ to carry out the structural optimization:

- The solid isotropic material with penalization (SIMP) scheme (Sigmund, 2001), with which the material property such as Young's modulus can be constructed as

$$E(\rho) = \rho^p E_0, \quad (1.1)$$

- The rational approximation of material properties (RAMP) scheme (Stolpe and Svanberg, 2001), which has a different form as

$$E(\rho) = \frac{\rho}{1 + q(1 - \rho)}, \quad (1.2)$$

where E_0 is the reference Young's modulus field; $p > 1$ and $q > 1$ are penalization factors for the SIMP and RAMP schemes, respectively.

Using the continuous density values, each element in the design domain is assigned a density variable ρ_e , where $\rho_e \in [0, 1]$. Specifically, $\rho_e = 1$ denotes solid material, $\rho_e = 0$ denotes void material, and those intermediate values ($0 < \rho_e < 1$) represent unclear material property between the solid and void materials, which will be penalized towards 0 or 1 during the optimization. In the numerical implementation, the minimum value of ρ_e is set as a small value (e.g., 10^{-3}) to avoid the numerical singularity.

The density method is highly regarded for its simplicity and broad applicability across a wide range of structural optimization problems, making it the preferred choice for topology optimization in most commercial software, such as Altair (www.altair.com) and COMSOL (www.comsol.com). Its penalization scheme effectively promotes near-binary designs, resulting in practical material distribution. Additionally, the density method's straightforward implementation further enhances its popularity in both academic and industrial applications.

However, the density method also has certain challenges. A key issue is the occurrence of intermediate densities, which persist despite the penalization effect. These intermediate densities have no physical meanings and often require post-processing to make the designs suitable for practical applications. Besides, the density method can result in a numerical phenomenon known as "checkerboard" (Shukla, Misra, and Kumar, 2013), cf. Fig. 1.1, which needs to be addressed using special techniques like sensitivity filtering. Furthermore, because the method operates on

a fixed mesh, the resulting designs often feature non-smooth structural boundaries, necessitating further refinement for real-world manufacturing.

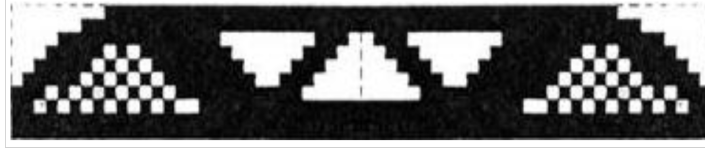


FIGURE 1.1: The checkerboard pattern obtained using the density method (Shukla, Misra, and Kumar, 2013).

1.2.2 Evolutionary method

The evolutionary method, commonly referred to as the evolutionary structural optimization (ESO) method, was proposed by Xie and Steven in the 1990s (Xie and Steven, 1993) and has been successfully applied in the modern architecture design, cf. Fig. 1.2. Unlike the density method, the ESO method uses binary design variables (i.e., $\rho_e = 0$ or 1) and slowly removes inefficient material from the design domain based on the von Mises stress distribution in its early version. Despite its simplicity, such a hard-kill scheme limits design freedom and may lead to local optima. To address this, a more advanced version called bi-directional ESO (BESO) method (Yang, Xie, Steven, and Querin, 1999; Querin, Young, Steven, and Xie, 2000) was later developed by the ESO group. Differently, the BESO method allows for both the removal and addition of materials simultaneously, improving flexibility and enhancing the optimization process.



FIGURE 1.2: Qatar national convention center (www.qncc.qa).

It should be noted that the original versions of ESO/BESO methods rely on a heuristic scheme to search for the optimal solution from a large set of solutions obtained during the TO process and the effectiveness of these methods is highly dependent on the tuning of specific parameters, which can significantly influence the quality and accuracy of the results. In 2010, Huang and Xie (Huang, Zuo, and Xie, 2010; Huang and Xie, 2010) introduced the rigorous optimality criteria into the BESO

updating scheme and proposed a soft-kill BESO approach with material interpolation scheme. This updated version of the BESO method demonstrates enhanced optimum searching capabilities and offers greater flexibility in addressing a wide range of engineering problems. Besides, it has been further refined and developed into the commercial software Ameba (<https://ameba.xieym.com/>). However, due to its reliance on a fixed discretized mesh of the design domain, the BESO method also requires the use of filtering techniques and other special approaches to deal with the potential “checkerboard” and zig-zag structural boundaries, similar to the design method but no intermediate densities need to be handled.

1.2.3 Level set method

Originally proposed by Osher and Sethian (Osher and Sethian, 1988), the level set (LS) method represents structural configurations in an implicit form using the iso-surfaces of a scalar LS function and has been introduced into structural TO in 2000 by Sethian and Wiegmann (Sethian and Wiegmann, 2000). The structural evolution is achieved with the movement of structural outlines by updating the LS function throughout the optimization process. As illustrated in Fig. 1.3, the material description using the LS function can be formulated as

$$\begin{cases} \phi(x) > 0 & \text{for } x \in \Omega \\ \phi(x) = 0 & \text{for } x \in \partial\Omega \\ \phi(x) < 0 & \text{for } x \in D \setminus \bar{\Omega} \end{cases} \quad (1.3)$$

where Ω denotes the material or fluid phase, D is the design domain, and $\partial\Omega$ represents the phase boundary. The expression $D \setminus \bar{\Omega}$ refers to the part of the design domain that excludes both the material/fluid phase and its boundary."

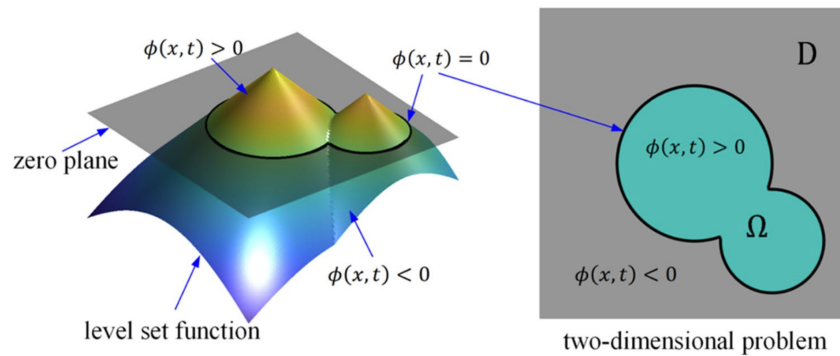


FIGURE 1.3: Level set description (Jiang and Zhao, 2022).

It should be noted that most LS methods are strictly shape optimization approaches as they move the shape of given structures. However, as structural boundaries evolve, the merging of holes can alter the topology. For this reason, LS methods are still widely regarded, to some extent, as TO methods. Till now, many different LS approaches have been proposed, such as discrete

LS method (Challis, 2010), filter-based LS method (Yaghmaei, Ghoddosian, and Khatibi, 2020), parameterized LS method (Li, Luo, Gao, and Wu, 2018; Luo, Wang, Wang, and Wei, 2008), and they have great advantages in many physical fields (e.g., fluid mechanics and phase transition).

Since the LS method uses the iso-surface of the LS function to describe the structural boundaries, the optimized results do not exhibit gray-scale or checkerboard patterns. Additionally, the structural boundaries depicted by the LS surface are always smooth, thus, the optimized designs do not require extra treatment for boundary smoothness and can be directly utilized in CAD modeling. However, several issues should still be considered for achieving optimal solutions and practical industrial applications. The biggest challenge with LS methods lies in their dependency on the initial design. While they allow the merging of holes, LS methods often lack the ability to nucleate new voids, which limits their capacity to explore the design space. Furthermore, re-initialization of the LS function and mesh dependency can introduce further numerical challenges.

1.3 Sensitivity analysis

Sensitivity information is crucial for these TO methods that use gradient-based optimizers. It provides the gradient of the given objective function with respect to design variables, which guides the direction of movement toward the optimal solution. In this section, we introduce two approaches for calculating sensitivity analysis: the direct difference method and the adjoint method. However, it should be noted that the finite difference method, another popular sensitivity analysis approach, is widely used in TO as well. A detailed derivation for calculating the shape derivative, which is commonly used in level set methods, is also provided.

1.3.1 Analysis approaches

For a better illustration and simplicity, here we consider a density-based stiffness optimization problem which can be mathematically constructed as

$$\begin{aligned} & \text{find } \rho_e, \quad e = 1, \dots, N, \\ & \min : c = \mathbf{F}^T \mathbf{U} = \mathbf{U}^T \mathbf{K} \mathbf{U} = \sum_e^N \mathbf{u}_e^T \mathbf{k}_e \mathbf{u}_e, \\ & \text{s.t. } \mathbf{K}(\rho) \mathbf{U} = \mathbf{F}, \end{aligned} \tag{1.4}$$

where ρ_e is the design variable of the e -th element, N denotes the total number of elements, $\mathbf{F}$ is the force vector, $\mathbf{U}$ is the displacement vector, and $\mathbf{K}$ is the global stiffness matrix.

Using the density method, the elemental stiffness matrix can be written as

$$\mathbf{k}_e(\rho_e) = (\rho_e)^p \mathbf{k}_0, \tag{1.5}$$

where $\mathbf{k}_0$ is the elemental stiffness matrix of a solid element.

Direct method

Using the direct method, the sensitivity can be calculated as

$$\frac{\partial c}{\partial \rho_e} = \frac{\partial (\mathbf{U}^T \mathbf{K} \mathbf{U})}{\partial \rho_e} = \frac{\partial \mathbf{U}^T}{\partial \rho_e} \mathbf{K} \mathbf{U} + \mathbf{U}^T \frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} + \mathbf{U}^T \mathbf{K} \frac{\partial \mathbf{U}}{\partial \rho_e} \quad (1.6)$$

Due to the state equation $\mathbf{K} \mathbf{U} = \mathbf{F}$ and the external force vector $\mathbf{F}$ has no relationship with the design variable, we take partial derivatives on both sides of the equilibrium and we have

$$\frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} + \mathbf{K} \frac{\partial \mathbf{U}}{\partial \rho_e} = 0. \quad (1.7)$$

Due to the symmetry characteristic of the stiffness matrix $\mathbf{K}$, the sensitivity equation Eq. (1.6) can be finally formulated as

$$\frac{\partial c}{\partial \rho_e} = -\mathbf{U}^T \frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} = -p(\rho_e)^{p-1} \mathbf{u}_e^T \mathbf{k}_0 \mathbf{u}_e. \quad (1.8)$$

Adjoint method

To calculate the sensitivity using the adjoint method, the Lagrangian L should be constructed with the Lagrangian multiplier (or the adjoint variable) λ as

$$L = c + \lambda^T (\mathbf{K} \mathbf{U} - \mathbf{F}). \quad (1.9)$$

Then, we calculate the partial derivative of L with respect to the design variable ρ_e and obtain the following formulation

$$\frac{\partial L}{\partial \rho_e} = \frac{\partial c}{\partial \rho_e} + \lambda^T \left(\frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} + \mathbf{K} \frac{\partial \mathbf{U}}{\partial \rho_e} - \frac{\partial \mathbf{F}}{\partial \rho_e} \right), \quad (1.10a)$$

$$= \frac{\partial F^T}{\partial \rho_e} \mathbf{U} + \mathbf{F}^T \frac{\partial \mathbf{U}^T}{\partial \rho_e} + \lambda^T \left(\frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} + \mathbf{K} \frac{\partial \mathbf{U}}{\partial \rho_e} - \frac{\partial \mathbf{F}}{\partial \rho_e} \right), \quad (1.10b)$$

$$= (\mathbf{F}^T + \lambda^T \mathbf{K}) \frac{\partial \mathbf{U}}{\partial \rho_e} + \lambda^T \frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U}. \quad (1.10c)$$

Assuming that $\mathbf{F}^T + \lambda^T \mathbf{K} = 0$, i.e., $\lambda = -\mathbf{K}^{-1} \mathbf{F} = -\mathbf{U}$, the following final formulation for the calculation of the sensitivity yields:

$$\frac{\partial L}{\partial \rho_e} = \lambda^T \frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} = -\mathbf{U}^T \frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U}, \quad (1.11a)$$

$$= -p(\rho_e)^{p-1} \mathbf{u}_e^T \mathbf{k}_0 \mathbf{u}_e. \quad (1.11b)$$

1.3.2 Derivation of the shape sensitivity

In this subsection, we describe the derivation of the shape derivative for the stiffness optimization problem in details. The mathematical model for the static TO process can be re-formulated as

$$\begin{aligned} \min : J &= \int_{\Omega} f u d\Omega + \int_{\Gamma_N} g u d\Gamma \\ \text{s.t. } \begin{cases} -\operatorname{div}(\mathbf{A} \mathbf{e}(\mathbf{u})) = f & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_D, \\ \mathbf{A} \mathbf{e}(\mathbf{u}) \cdot \mathbf{n} = 0 & \text{on } \Gamma_N, \end{cases} \end{aligned} \quad (1.12)$$

Therefore, the Lagrangian equation can be constructed using the Lagrange multipliers as follows:

$$L = J + \int_{\Omega} \lambda_1 (-\operatorname{div}(\mathbf{A} \mathbf{e}(\mathbf{u})) - f) d\Omega + \int_{\Gamma_D} \lambda_2 (\mathbf{u} - 0) d\Gamma + \int_{\Gamma_N} \lambda_3 (\mathbf{A} \mathbf{e}(\mathbf{u}) \cdot \mathbf{n} - g) d\Gamma. \quad (1.13)$$

According to the optimality theory, we assume that the optimal point of the considered problem is $L(w, p, \Omega)$, which means

$$\left\langle \frac{\partial L}{\partial w}, \delta w \right\rangle = 0 \Leftrightarrow \frac{\partial L}{\partial w} = 0. \quad (1.14)$$

Then, we have

$$\begin{aligned} \frac{\partial L}{\partial w} &= \int_{\Omega} f \delta w d\Omega + \int_{\Gamma_N} g \delta w d\Gamma - \left(\int_{\Gamma} \lambda_1 \mathbf{A} \mathbf{e}(\delta w) \cdot \mathbf{n} d\Gamma - \int_{\Omega} e(\lambda_1) \mathbf{A} \mathbf{e}(\delta w) d\Omega \right) \\ &\quad + \int_{\Gamma_D} \lambda_2 \delta w d\Gamma + \int_{\Gamma_N} \lambda_3 \mathbf{A} \mathbf{e}(\delta w) \cdot \mathbf{n} d\Gamma \end{aligned} \quad (1.15a)$$

$$\begin{aligned} &= \int_{\Omega} f \delta w d\Omega + \int_{\Gamma_N} g \delta w d\Gamma - \int_{\Gamma} \lambda_1 \mathbf{A} \mathbf{e}(\delta w) \cdot \mathbf{n} d\Gamma + \int_{\Gamma} \delta w \mathbf{A} \mathbf{e}(\lambda_1) \cdot \mathbf{n} d\Gamma \\ &\quad - \int_{\Omega} \operatorname{div}(\mathbf{A} \mathbf{e}(\lambda_1)) \delta w d\Omega + \int_{\Gamma_D} \lambda_2 \delta w d\Gamma + \int_{\Gamma_N} \lambda_3 \mathbf{A} \mathbf{e}(\delta w) \cdot \mathbf{n} d\Gamma. \end{aligned} \quad (1.15b)$$

Using the integration by parts as follows

$$\int_{\Omega} \operatorname{div}(\mathbf{A}e(\mathbf{u}))\lambda d\Omega = \int_{\Gamma} \mathbf{A}e(\mathbf{u})\lambda \cdot \mathbf{n} d\Gamma - \int_{\Omega} e(\lambda)\mathbf{A}e(\mathbf{u})d\Omega, \quad (1.16a)$$

$$\int_{\Omega} \mathbf{A}e(\mathbf{u})e(\lambda)d\Omega = \int_{\Gamma} \lambda\mathbf{A}e(\mathbf{u}) \cdot \mathbf{n} d\Gamma - \int_{\Omega} \operatorname{div}(\mathbf{A}e(\mathbf{u}))\lambda d\Omega. \quad (1.16b)$$

Eq. (1.15b) can be further derived as the following equation:

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{w}} = & \int_{\Omega} [\mathbf{f} - \operatorname{div}(\mathbf{A}e(\lambda_1))] \delta \mathbf{w} d\Omega + \int_{\Gamma_N} [\mathbf{g} + \mathbf{A}e(\lambda_1) \cdot \mathbf{n}] \delta \mathbf{w} d\Gamma + \int_{\Gamma_N} [(\lambda_3 - \lambda_1) \mathbf{A}e(\delta \mathbf{w}) \cdot \mathbf{n}] d\Gamma \\ & + \int_{\Gamma_D} [\lambda_2 + \mathbf{A}e(\lambda_1) \cdot \mathbf{n}] \delta \mathbf{w} d\Gamma - \int_{\Gamma_D} \lambda_1 \mathbf{A}e(\delta \mathbf{w}) \cdot \mathbf{n} d\Gamma. \end{aligned} \quad (1.17)$$

To make the above equation equal to 0, we have the following equations

$$\text{in } \Omega : \mathbf{f} - \operatorname{div}(\mathbf{A}e(\lambda_1)) = 0, \quad (1.18a)$$

$$\text{on } \Gamma_N : \mathbf{g} + \mathbf{A}e(\lambda_1) \cdot \mathbf{n} = 0 \Rightarrow \lambda_3 - \lambda_1 = 0, \quad (1.18b)$$

$$\text{on } \Gamma_D : \lambda_2 + \mathbf{A}e(\lambda_1) \cdot \mathbf{n} = 0 \Rightarrow \lambda_1 = 0. \quad (1.18c)$$

Therefore, we have the following relationships which indicates the self-adjoint characteristic of the stiffness optimization problem.

$$\lambda_1 = -\mathbf{u}, \lambda_2 = \mathbf{A}e(\mathbf{u}) \cdot \mathbf{n}, \lambda_3 = -\mathbf{u}. \quad (1.19)$$

As a result, the Lagrangian equation Eq. (1.14) can be newly written as

$$\begin{aligned} L = & \int_{\Omega} \mathbf{f} \mathbf{u} d\Omega + \int_{\Gamma_N} \mathbf{g} \mathbf{u} d\Gamma + \int_{\Omega} \mathbf{u} (\operatorname{div}(\mathbf{A}e(\mathbf{u})) + \mathbf{f}) d\Omega + \int_{\Gamma_D} \mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma \\ & - \int_{\Gamma_N} \mathbf{u} (\mathbf{A}e(\mathbf{u}) \cdot \mathbf{n} - \mathbf{g}) d\Gamma, \end{aligned} \quad (1.20a)$$

$$\begin{aligned} = & \int_{\Omega} 2\mathbf{f} \mathbf{u} d\Omega + \int_{\Gamma_N} \mathbf{g} \mathbf{u} d\Gamma + \int_{\Gamma} \mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma - \int_{\Omega} e(\mathbf{u}) \mathbf{A}e(\mathbf{u}) d\Omega \\ & + \int_{\Gamma_D} \mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma - \int_{\Gamma_N} \mathbf{u} (\mathbf{A}e(\mathbf{u}) \cdot \mathbf{n} - \mathbf{g}) d\Gamma, \end{aligned} \quad (1.20b)$$

$$\begin{aligned} = & \int_{\Omega} 2\mathbf{f} \mathbf{u} d\Omega + \int_{\Gamma_N} \mathbf{g} \mathbf{u} d\Gamma + \int_{\Gamma_N} \mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma + \int_{\Gamma_D} \mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma - \int_{\Omega} e(\mathbf{u}) \mathbf{A}e(\mathbf{u}) d\Omega \\ & + \int_{\Gamma_D} \mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma - \int_{\Gamma_N} \mathbf{u} (\mathbf{A}e(\mathbf{u}) \cdot \mathbf{n} - \mathbf{g}) d\Gamma, \end{aligned} \quad (1.20c)$$

$$= \int_{\Omega} 2\mathbf{f} \mathbf{u} d\Omega + \int_{\Gamma_N} 2\mathbf{g} \mathbf{u} d\Gamma + \int_{\Gamma_D} 2\mathbf{A}e(\mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma - \int_{\Omega} e(\mathbf{u}) \mathbf{A}e(\mathbf{u}) d\Omega. \quad (1.20d)$$

In the remarkable research work of (Allaire, Bonnetier, Francfort, and Jouve, 1997), two different forms of integration, i.e., domain and boundary integrations, are introduced as follows

$$\begin{aligned} \text{Domain integration: } J(\Omega) = \int_{\Omega} \boldsymbol{\phi}(x) dx &\Rightarrow J'(\Omega)(\boldsymbol{\theta}) = \int_{\Omega} \operatorname{div}(\boldsymbol{\theta}(x) \boldsymbol{\phi}(x)) dx \\ &= \int_{\partial\Omega} \boldsymbol{\theta}(x) \cdot \mathbf{n}(x) \boldsymbol{\phi}(x) ds, \end{aligned} \quad (1.21a)$$

$$\text{Boundary integration: } J(\Omega) = \int_{\partial\Omega} \boldsymbol{\phi}(x) ds \Rightarrow J'(\Omega)(\boldsymbol{\theta}) = \int_{\partial\Omega} \boldsymbol{\theta} \cdot \mathbf{n} \left(\frac{\partial \boldsymbol{\phi}}{\partial \mathbf{n}} + \mathbf{H} \boldsymbol{\phi} \right) ds, \quad (1.21b)$$

where $\boldsymbol{\theta}$ is the perturbation of the structural shape and $\mathbf{H}$ is mean curvature of the boundary.

Then, we can obtain the following formulation

$$\begin{aligned} L'(\Omega)(\boldsymbol{\theta}) = & \int_{\partial\Omega} 2\mathbf{f}\mathbf{u}\boldsymbol{\theta} \cdot \mathbf{n} d\Gamma - \int_{\partial\Omega} \mathbf{A}\mathbf{e}(\mathbf{u})\mathbf{e}(\mathbf{u})\boldsymbol{\theta} \cdot \mathbf{n} d\Gamma + 2 \int_{\Gamma_N} \left(\frac{\partial(\mathbf{g}\mathbf{u})}{\partial \mathbf{n}} + \mathbf{H}(\mathbf{g}\mathbf{u}) \right) \boldsymbol{\theta} \cdot \mathbf{n} d\Gamma \\ & + \int_{\Gamma_D} \mathbf{A}\mathbf{e}(\mathbf{u})\mathbf{e}(\mathbf{u})\boldsymbol{\theta} \cdot \mathbf{n} d\Gamma, \quad \mathbf{H} = \nabla \cdot \mathbf{n}. \end{aligned} \quad (1.22)$$

Because the boundaries are fixed during the optimization, the corresponding terms can be deleted. Using $\boldsymbol{\theta} \cdot \mathbf{n} = V^n$ on $\partial\Omega$ and the following equation,

$$\int_{\partial\Omega} f(x) dx = \int_{\Omega} f(x) \delta(\boldsymbol{\phi}(x)) |\nabla \boldsymbol{\phi}(x)| d\Omega, \quad (1.23)$$

the final shape derivative for the stiffness TO can be formulated as

$$J'(\Omega)(\boldsymbol{\theta}) = \int_{\Omega} [2\mathbf{f}\mathbf{u} - \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D} : \boldsymbol{\varepsilon}(\mathbf{u})] \delta(\boldsymbol{\phi}) |\nabla \boldsymbol{\phi}| V^n d\Omega. \quad (1.24)$$

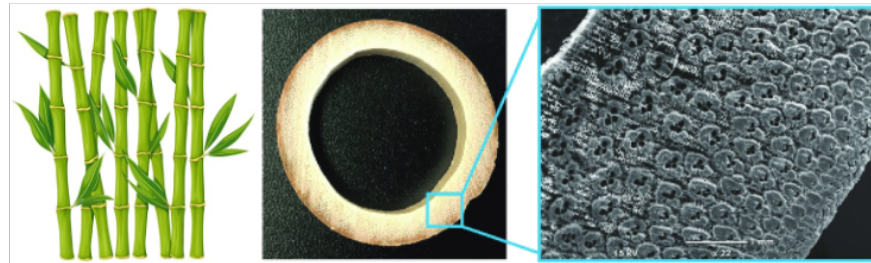
1.4 Research motivation

With the rapid development of modern manufacturing technologies (such as multi-axis milling and Stereolithography), TO is no longer limited to single-scale structures. Instead, it is evolving towards multiscale optimization, encompassing macroscale, microscale, even nanoscale. Among them, coated structures inspired by biological structures in nature (such as bird beaks and bamboo, cf. Fig. 1.4), have increasingly become a focal point in the multiscale TO and has been widely studied among the TO community. Besides, not only constrained by the academic study, many practical applications of coated structures also emerge in the industrial field. For instance, Adidas transplants the coated structure concept to running shoe design and optimized the midsole with lattice structures, cf. Fig. 1.5a, using two decades of high-speed motion capture and force data from nearly 4,000 runners. Aerojet Rocketdyne infilled the substrate of the “Mark II” injector block with self-supporting lattice microstructures, cf. Fig. 1.5b, whose weight has been reduced by 67% with doubled factor of safety. Although advances have moved beyond the single scale, most recent research and industrial applications in the optimal design of coated structures using TO

technique remain focused on the periodic and uniform distribution of a specific microstructural configuration. Consequently, further research is necessary to fully explore the potential of coated structures.



(A) Horbill bird beak.



(B) Bamboo.

FIGURE 1.4: Cross-sectional view of coated structures in the natural kingdom: (a) Horbill bird beak (Aage, Andreassen, Lazarov, and Sigmund, 2017); (b) bamboo (Sato, Inoue, and Shima, 2017).

Dynamic structural performance is a critical mechanical property of structures, significantly influencing the operational performance, effectiveness, and safety of both structures and mechanical systems. Absent or inadequate attention towards dynamic performance has led to numerous engineering failures, including the most well-known case that the resonance-induced collapse of the Tacoma narrows bridge. In the academia, most research works on the optimum design of coated structures focus on static structural performance, with relatively few studies addressing dynamic performance. This limitation hampers the application of advanced TO approaches in real-world engineering scenarios, and stimulates my passion on studying multiscale TO of coated structures considering dynamic structural performance.

Multimaterial TO is also an increasing popular trend which considers the optimal distribution of multiple materials for achieving better structural performance or specific functionalities. Exhibiting more potential than single material case, practical engineering designs usually incorporate a variety of materials, such as combining composite materials (e.g., carbon fiber and fiberglass) with metals in wind turbines to balance structural strength, durability, and lightweight properties. While significant progress has been made in multimaterial TO, few studies specifically address multimaterial coated structures. The presence of an outer coating allows greater flexibility



(A) Adidas shoe.



(B) "Mark II" injector block.

FIGURE 1.5: Practical industrial applications of coated structures: (a) Adidas shoe (www.ntop.com) and (b) "Mark II" injector block (www.carbon3d.com) infilled with lattice microstructures.

in using various materials as infills, as the coating ensures structural integrity, reducing concerns about the connectivity between different materials.

Microstructures with varying topologies demonstrate distinct homogenized material properties. Exploiting the advantages of microstructures, TO of multi-material structures composed of optimized microstructural configurations has gained increasing attention in the TO community. However, there has been limited progress in designing the optimal distribution of multiple materials within coated structures. Inspired by natural coated structures with non-homogeneous microstructures, exploring the integration of diverse microstructural configurations within the coating presents an exciting opportunity. The introduction of multiple microstructures as the infilling for coated structures can improve structural performance while preserving lightweight properties, which is pretty attractive for industrial applications.

Despite significant attention from academia and industry, the design of coated structures typically assumes an external coating of uniform thickness. While this approach has led to notable advancements, coated structures in nature often display varied coating thicknesses to better withstand external loads or stimuli. For instance, as shown in Fig. 1.6, the human bone's coating at the base is significantly thicker than in other regions, highlighting the advantages of non-uniform coatings. Thus, TO for the design of coated structures with variable thickness is expected to offer greater design flexibility and improved performance compared to those with uniform coatings. To

further explore the natural growth strategies and investigate the potential of coated structures, we aim to achieve variable coating designs through numerical algorithms using the TO technique. Besides, with the popularity of adding body-fitted mesh into the TO process, how to generate smooth structural boundaries using the density method is also of my great interest.

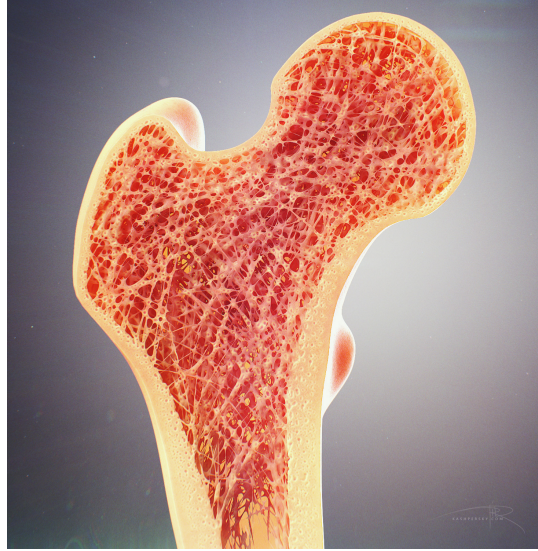


FIGURE 1.6: Cross-sectional view of a human bone with variable coating thickness (www.kashpersky.com).

1.5 Outline of the thesis

This thesis is devoted to developing innovative and efficient optimum design methods for coated structures, with the goal of developing their potential and facilitating their practical application in real-world industrial settings. We aim to establish both the theoretical foundations and computational frameworks necessary for the design of coated structures considering multiple scales, multiple materials, and non-uniform coating thickness, utilizing LS and density methods.

In Chapter 2, we focus on maximizing the eigenfrequency of coated structures filled with inhomogeneous lattice microstructural infilling. Getting inspiration from functionally graded materials, the infilling of coated structures is divided into multiple layers, with each composed of different optimized microstructural configurations. A novel multiscale TO framework is developed, combining the VFLS method with the widely used SIMP method. This chapter provides a detailed introduction to the VFLS method, along with the mathematical model for the eigenfrequency maximization problem. To handle multiple eigenfrequencies, the modal assurance criterion (MAC) approach is employed and its effectiveness is demonstrated. The impact of various factors, such as the number of divided layers and varying coating thicknesses, on the optimization results is examined through several numerical examples. Finally, the manufacturability of the

optimized coated structures is assessed, confirming the effectiveness of the proposed multiscale TO framework.

In Chapter 3, the previously developed TO framework for the optimal design of multiscale coated structures is extended to address the dynamic compliance minimization problem. Considering time-harmonic excitation at a specific frequency, a mathematical model is constructed for minimizing the dynamic compliance of coated structures infilled with layer-wise lattice microstructures. In addition to two volume constraints at two scales, a static compliance constraint is introduced to ensure the material connectivity under ‘high’ excitation frequencies. Furthermore, the infilling microstructures are designed as bi-material lattice microstructures using the SIMP method. Compared to single-material designs, bi-material microstructures are expected to offer superior performance, particularly towards dynamic structural performance. Through various numerical examples, the effects of different excitation frequencies, damping coefficients, coating thicknesses, etc., are analyzed, confirming the effectiveness of the proposed method.

In Chapter 4, we shed a light on the optimal design of coated structures filled with multiple materials using TO. To develop an easy-to-use method, a new ordered SIMP-based approach is proposed, incorporating commonly used filtering and projection operations. Notably, a ‘strict’ Heaviside projection is introduced for the identification of the external coating during the TO process. Leveraging the benefits of the original ordered SIMP approach, the proposed method operates with a single density variable field and demonstrates stable iteration behavior. The coating, substrate, and distribution of various infilling materials within the coated structures are represented through multiple filtered fields, allowing for implicit control over the coating thickness. Several 2D numerical examples, along with a 3D example, are presented to validate the effectiveness of the proposed method and highlight its advantages.

In Chapter 5, we return to the multiscale design of coated structures. Unlike previous studies, we explore multiscale structural design by extending the concept of multimaterial TO and develop a new multiscale TO approach for coated structures filled with multiple self-connected microstructures. Specifically, the infill of the coated structures consists of various types of microstructural configurations. Due to their differing macroscale material properties, this distribution can be treated as a multimaterial optimization problem. Building upon the previously developed ordered SIMP scheme, the macroscale structural layout with multiple infilling material blocks is determined using several modified density fields. Subsequently, distinct lattice microstructures are optimized and assigned to corresponding material blocks, with their material properties calculated through the homogenization method. To ensure connectivity between microstructures across neighboring material blocks, the designable connective region (DCR) method is introduced, allowing for well-connected microstructures and achieving self-connectivity. The effectiveness of the proposed method is demonstrated, with discussions on the impact of factors such as coating thickness and the number of microstructures. Finally, the manufacturability of

optimized coated structures with self-connected microstructures is validated using additive manufacturing techniques.

In Chapter 6, we target on further developing the potential of coated structures by proposing a novel TO method for designing coated structures with non-uniform coating thickness. Utilizing the density method, the smoothing filter radius is selected as a design variable and optimized concurrently with the density field. As the structural topology evolves, the coating thickness is implicitly updated during the optimization process to enhance resistance to external forces. Additionally, an improved partial differential equation (PDE) filter with a non-homogeneous Neumann boundary condition is introduced to simplify the modeling process. Compared to the case of uniform coating, the advantages of using non-uniform coating thickness are demonstrated. The classical stiffness maximization problem is examined with several numerical examples to assess the effectiveness, practicality, and flexibility of the proposed approach.

In Chapters 2 to 6, we first present an in-depth literature review relevant to the topic of each chapter. Next, the main challenges and innovative aspects of the research are introduced. Following that, the key techniques of the proposed TO methods or frameworks are explained, with mathematical models constructed to support the approaches. Sensitivity analysis formulations are provided in subsequent sections, followed by numerical examples that demonstrate the effectiveness of the developed methods. Finally, concluding remarks and discussions are summarized at the end of each chapter.

Chapter 2

Multiscale topology optimization of coated structures for maximizing the fundamental eigenfrequency[†]

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2.1 Introduction

Being an innovative structural configuration, a coated structure (or shell-infill structure) is composed of an outer coating and an interior substrate. Functionally, the outer coating provides protection to the substrate of coated structures and can improve some structural functionalities. Lattice structures, which is usually made of periodic and uniform microstructures, are promising and ideal to be used as the substrate of coated structures thanks to their extraordinary physical and mechanical performances, such as high strength-to-weight ratio and superior energy absorption ability. Besides, experiments show that coated structures with lattice infill exhibits higher performance of buckling resistance (Clausen, Aage, and Sigmund, 2016). Attracting great interest from academia and industry, coated structures with lattice infill have exhibited great potential in many applications such as medical implant (Heimann and Lehmann, 2015), vibration mitigation (Matlack, Bauhofer, Krödel, Palermo, and Daraio, 2016), and heat conduction (Cheng, Liu, and To, 2018).

As is well-known, topology optimization (TO) has a high design flexibility to find an optimal configuration that can maximize the objective under a given set of constraints. It has been widely applied to solve various optimum design problems such as reinforcement optimization (Wang and Abdalla, 2015; Hu, Ding, Shen, and Zhang, 2020; Hu, Ding, Zhang, Shen, and Li, 2023), composite material design (Sigmund and Torquato, 1999; Zhang, Ding, Wang, Ni, and Li, 2020), thermal fluid-structure system design (Li, Kondoh, Jolivet, Furuta, Yamada, Zhu, Izui, and Nishiwaki, 2022; Li, Kondoh, Jolivet, Furuta, Yamada, Zhu, Zhang, Izui, and Nishiwaki, 2022), and thermoelastic structure optimization (Fang, Wang, and Zhou, 2022). Various topology optimization methods have been proposed since the pioneering work of Bendsøe and Kikuchi (Bendsøe and Kikuchi, 1988), including the solid isotropic material with penalization method (SIMP) (Bendsøe, 1989; Bendsøe and Sigmund, 1999), the evolutionary structural optimization method (ESO)/bidirectional ESO method (BESO) (Xie and Steven, 1993; Huang, Xie, and Burry, 2006), level set method (LSM) (Allaire, Jouve, and Toader, 2002; Wang, Wang, and Guo, 2003), and feature driven methods such as the moving morphable component method (MMC) approach (Guo, Zhang, and Zhong, 2014), moving morphable void (MMV) approach (Zhang, Chen, Zhu, Zhou, Xue, Lei, and Guo, 2017) and moving wide bezier components with constrained ends (Zhu, Wang, Wang, Li, Zhang, and Nishiwaki, 2021) over decades of research. Recently, with the rapid development of additive manufacturing (AM) technique, topology optimization has undergone vigorous research activities for the possible fabrication of optimized novel structural configurations using the AM.

Many research works have been carried out towards topology optimization of coated structures with porous or lattice infill (Wu, Aage, Westermann, and Sigmund, 2017; Liu, Zhou, Wei, and Lin, 2021; Wang and Kang, 2018a; Fu, Li, Xiao, Gao, and Chu, 2019; Clausen, Andreassen, and Sigmund, 2017). However, some of them only focused on the microscale topology optimization whereas the macrostructure is predefined. Although reasonable structures can be generated in this way to improve mechanical performance, the macroscale outer coating with a uniform (or

non-uniform) thickness of coated structures have direct influence on the porous or lattice infill at microscale and vice versa (Fu, Li, Gao, and Xiao, 2019). Therefore, multiscale topology optimization is the most suitable way for the design of coated structures filled with lattice infill due to its thoughtful consideration of the interaction between the material distribution at different scales. Wadbro and Niu (Wadbro and Niu, 2019) introduced harmonic-mean based non-linear filters into the porous anisotropic material with penalization (PAMP) method to identify the coating and optimized coated structures with periodic infill pattern. Different from the density-based approaches, the level-set based methods are free of the filtering, projection, or gradient norm approaches, but can still identify the coating of uniform thickness using a signed distance function. More accurately speaking, only two distinct level set surfaces of one single level set function need to be used to describe the domain of the shell, the infill, and their interface. In the research of Fu et al. (Fu, Li, Gao, and Xiao, 2019), a multiscale level set topology optimization method was proposed to solve a mean compliance problem. They simultaneously optimized the shell and the lattice infill using the parametric level set method. Jiang et al. (Jiang, Guo, Chen, Wei, Lei, and Gu, 2019) performed concurrent optimization of structural topology and infill properties based on a cardinal basis function-based level set method. Some other works used BESO method. For example, Qiu et al. (Qiu, Jin, Jin, Wang, Xia, Zhu, and Shi, 2020) proposed a two-step evolutionary design procedure, in which the macroscale structural configuration was firstly designed with a weaker homogeneous material filled in, and then the lattice infill architecture was generated under a maximum length scale constraint.

To some extent, coated structures with lattice infill show similar features with those found in the natural world (e.g., honeycomb, bird beak, bone, bamboo, etc.). However, it has been pointed out by (Miyamoto, Kaysser, Rabin, Kawasaki, and Ford, 2013; Coelho, Fernandes, Rodrigues, Cardoso, and Guedes, 2009) that the infill of these biological structures found in the nature are usually inhomogeneous and spatially varied to adapt to their environmental stimuli. This can be considered as the origin of the functionally graded material. Compared to the periodic and homogeneous microstructures, functionally graded lattice structures can take the advantages of both lattice infill and graded materials. Groen et al. (Groen, Wu, and Sigmund, 2019) proposed a homogenization-based topology optimization method for coated structures with orthotropic infill structures. Following Groen's approach, Lee et al. (Lee, Kwon, Yoo, Min, Nomura, and Dede, 2021) designed coated structures with spatially-varying orthotropic infill material using a de-homogenization process and explicit structural representation can be achieved with the projection approach based on the implicit mapping function. Chu et al. (Chu, Gao, Xiao, and Zhang, 2020) investigated topology optimization of coated structures with multifarious-microstructural infill, in which controllable kinds of microstructures are generated to be the infill by pre-defining several volume fractions. Another novel approach to achieve graded materials is to design lattice compromising multiple layers of periodic microstructures. Zhang and Sun (Zhang and Sun, 2006) studied 2D multi-layer structures composed of intermediate macroscale elements assigned with different microstructures. Li et al. (Li, Luo, Gao, and Walker, 2018) presented macrostructures with functionally graded layer-wise cellular composites hosting auxetic metamaterials. Zhang

et al. (Zhang, Wang, and Kang, 2019) proposed concurrent multiscale topology optimization of structures composed of layer-wise graded lattice microstructures, in which the design of bi-material graded lattice structures was also considered.

In contrast to the mean compliance problem, the dynamic topology optimization has received much less attention in the context of coated structures embedded with the lattice infill, despite the consensus of the importance of dynamic structural performance (Li, Sigmund, Jensen, and Aage, 2021). Generally, the existed works on dynamic topology optimization mainly focus on two aspects. One is to minimize the dynamic response (Shen, Ding, Hu, Xiong, and Zhang, 2021). For example, Zhang and Kang (Zhang and Kang, 2014) firstly proposed a generic topology optimization formulation for the vibrating structures under transient dynamic loads, and then a single-loop robust topology optimization method that can efficiently handle dynamic load uncertainty was proposed by Zhang et al (Zhang, Kang, and Zhang, 2016). Niu and Wadbro (Niu and Wadbro, 2021) proposed an optimization strategy to minimize the dynamic compliance of vibrating shell-infill structures, in which macroscale structures and their periodic uniform lattice infill were concurrently designed. The other challenging one is the maximization of eigenfrequencies. For instance, Du and Olhoff (Du and Olhoff, 2007) treated topology optimization of freely vibrating continuum structures considering simple and multiple eigenfrequencies. Pedersen (Pedersen, 2000) studied the efficiency of several different SIMP models and maximized the fundamental eigenfrequency of plates. Xie and Steven (Xie and Steven, 1996) extended the ESO method to the maximization of structural eigenfrequencies. Xia et al. (Xia, Shi, and Wang, 2011) proposed a level set based shape and topology optimization method and maximized the simple (or repeated first) eigenvalue of structures. Although maximizing eigenfrequencies of structures is always a popular topic among the field of TO, to this date, very few research has conducted multiscale topology optimization of coated structures with lattice infill for the maximization of eigenfrequencies to the best of our knowledge.

In this work, we aim to develop a novel framework for the concurrent multiscale topology optimization of coated structures embedded with layer-wise graded lattice infill to maximize the fundamental eigenfrequency. Topologies of macroscale structures and layer-wise lattice infill are determined by macroscale and microscale design variables, respectively. At microscale, the infill lattice structures are divided into several layers, which are determined by different microscale design variables. The conventional SIMP method is used to optimize the lattice infill for different layers, subjected to a microscale total volume constraint. At macroscale, the velocity field-based level set (VFLS) method (Wang and Kang, 2018b; Wang and Kang, 2021) is employed to generate a binary structure. Two level set surfaces of one single level set function are utilized to model the coating. The influence of divided layers for the lattice infill and thickness of the outer coating on the topological design of coated structures with graded layer-wise microstructures are studied through several numerical examples.

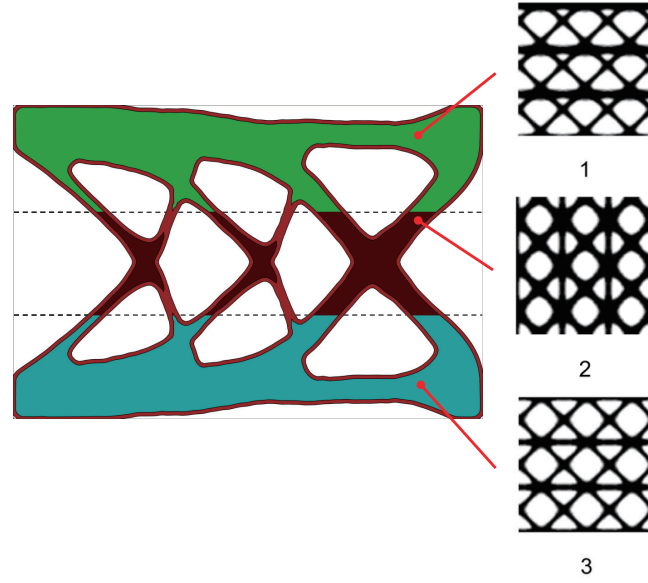


FIGURE 2.1: Schematic illustration of a coated structure with layer-wise graded lattice infill.

The remaining of this paper is organized as follows. Section 2.2 introduces the multiscale design model of coated structures with graded layer-wise lattice infill. Section 2.3 presents the optimization formulation and in Section 2.4 we derive the sensitivity analysis at two scales. The effectiveness of the proposed framework is demonstrated with numerical examples in Section 2.5, and several 3D printed prototypes are manufactured. Finally, Section 2.6 concludes the paper.

2.2 Multiscale topology optimization model

Fig. 2.1 schematically illustrates the configuration of a coated structure filled with multi-layer graded lattice infill. At the macro scale, the outer coating has a uniform thickness and is presented in red. The substrate regions for different lattice infill layout are marked in different colors, see the three zoom views on the right. For each layer, the lattice infill are all assumed to have periodic lattice structures. The optimized microstructural configurations are all presented in a 3-by-3 repetition form. In the figures of microstructures, the white domain represents the void and the black domain represents the solid. The numbering of layers for the lattice infill is given from top to bottom.

2.2.1 Microscale optimization based on SIMP method

In the proposed framework, we select the popular SIMP method to find optimal topologies of the lattice infill and use η to describe the density field of elements at the microscale. Physically,

$\eta = 1$ denotes solid phase and $\eta = 0$ denotes void phase. To avoid the numerical singularities, the minimum value of η in the SIMP method is set to a small positive value (e.g., 10^{-3}). Besides, in order to calculate the effective elasticity matrix of a unit cell, the size of a microscale element should be much smaller than that of a macroscale element. Microscale design variables within a unit cell k of a specific layer l can be expressed as follows:

$$\boldsymbol{\eta}_{l,k} = \left\{ \eta_{l,k}^1, \eta_{l,k}^2, \dots, \eta_{l,k}^{n^{\text{MI}}} \right\}^T, \quad l = 1, 2, \dots, L; \quad k = 1, 2, \dots, n_l^{\text{MA}}, \quad (2.1)$$

where n^{MI} is the number of finite elements discretized within a unit cell; n_l^{MA} is the number of unit cells of the l -th layer and L is the total number of divided layers for graded lattice infill.

Therefore, the microscale design variables collected within a single vector is

$$\boldsymbol{\eta} = \left\{ \boldsymbol{\eta}_{1,1}^T, \dots, \boldsymbol{\eta}_{1,n_1^{\text{MA}}}^T, \boldsymbol{\eta}_{2,1}^T, \dots, \boldsymbol{\eta}_{2,n_2^{\text{MA}}}^T, \dots, \boldsymbol{\eta}_{L,1}^T, \dots, \boldsymbol{\eta}_{L,n_L^{\text{MA}}}^T \right\}^T. \quad (2.2)$$

Using the asymptotic homogenization method (HassaniB, 1998), the effective elasticity matrix of a unit cell for 2D structures can be computed by

$$\mathbf{D}_{ijpq}^{\text{H}} = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} \mathbf{D}_{rskt}^{\text{MI}} \left(\boldsymbol{\varepsilon}_{rs}^{0(ij)} - \boldsymbol{\varepsilon}_{rs}^* \left(\boldsymbol{\chi}^{ij} \right) \right) \left(\boldsymbol{\varepsilon}_{kt}^{0(pq)} - \boldsymbol{\varepsilon}_{kt}^* \left(\boldsymbol{\chi}^{pq} \right) \right) d\mathbf{y}, \quad i, j, p, q = 1, 2, \quad (2.3)$$

where $\mathbf{D}_{rskt}^{\text{MI}}$ is the elasticity matrix of the base material of microstructures; $|\mathbf{Y}|$ denotes the volume of a unit cell, and $\boldsymbol{\chi}$ is the characteristic microscale displacement field of the unit cell; In the 2D case, the applied test strain fields $\boldsymbol{\varepsilon}_{rs}^{0(ij)}$ include the horizontal unit strain $\boldsymbol{\varepsilon}_{rs}^{0(11)} = [1, 0, 0]^T$, the vertical unit strain $\boldsymbol{\varepsilon}_{rs}^{0(22)} = [0, 1, 0]^T$, and the shear unit strain $\boldsymbol{\varepsilon}_{rs}^{0(12)} = [0, 0, 1]^T$; $\boldsymbol{\varepsilon}_{rs}^* \left(\boldsymbol{\chi}^{ij} \right)$ refers to the varying strains.

For the material interpolation at the microscale, we follow Wadbro and Niu (Wadbro and Niu, 2019). The Young's modulus and material density are interpolated as follows:

$$E_s(\eta) = E_{\min} + (E_0 - E_{\min}) \eta^{\xi}, \quad (2.4a)$$

$$\rho_s(\eta) = \rho_{\min} + (\rho_0 - \rho_{\min}) \eta, \quad (2.4b)$$

where $E_{\min}$ and $\rho_{\min}$ are set to small positive values for the void region, respectively; E_0 and ρ_0 are the Young's modulus and the material density of the base material, respectively; ξ is the penalty factor, which is often set to be larger or equal to 3 (Bendsøe and Sigmund, 1999) and is given as 3 in this study. The numerical examples presented in this paper all use $E_{\min} = 10^{-3}E_0$ and $\rho_{\min} = 10^{-3}\rho_0$.

Therefore, the elasticity matrix of a microscale element has the following form:

$$\mathbf{D}_{rskt}^{\text{MI}} = E_s(\eta) \mathbf{D}_{rskt}^0 = \left(E_{\min} + (E_0 - E_{\min}) \eta^{\xi} \right) \mathbf{D}_{rskt}^0, \quad (2.5)$$

where $\mathbf{D}_{rskt}^0$ and E_0 are the dimensionless isotropic elasticity matrix and Young's modulus of the base material, respectively.

By applying the test strain fields, the varying strains $\epsilon_{rs}^* (\chi^{ij})$ induced by $\epsilon_{rs}^{0(ij)}$ can be calculated by

$$\epsilon_{rs}^* (\chi^{ij}) = \frac{1}{2} (\chi_{r,s}^{ij} + \chi_{s,r}^{ij}). \quad (2.6)$$

Here, the characteristic displacement field χ^{ij} can be obtained by solving the following microscale problem:

$$\int_{\mathbf{Y}} \mathbf{D}_{rskt}^{\text{MI}} (\epsilon_{rs}^* (\chi^{ij}) - \epsilon_{rs}^0 (\chi^{ij})) \epsilon_{kt} (\delta^{pq}) \, d\mathbf{y} = 0, \quad \forall \delta \in U(\mathbf{Y}), \quad (2.7)$$

where δ^{pq} is the virtual displacement field and $U(\mathbf{Y})$ is the set of all the kinematically admissible displacements in $\mathbf{Y}$.

2.2.2 Macroscale optimization based on velocity field-based level set method

Velocity field-based level set method

In this subsection, we will recall the basic concept of the VFLS method and readers can refer to the publication of one of the authors (Wang and Kang, 2018b; Wang and Kang, 2021) for more details.

Inheriting the implicit representation of structural topology, the VFLS method can describe a coated structure with an outer coating of uniform thickness using only one single level set function (Wang and Kang, 2018a) as follows:

$$\left\{ \begin{array}{ll} \phi(\mathbf{x}) < 0, & \mathbf{x} \in \Omega_v, \\ \phi(\mathbf{x}) = 0, & \mathbf{x} \in \Gamma_{cv}, \\ 0 < \phi(\mathbf{x}) < b_c, & \mathbf{x} \in \Omega_c, \\ \phi(\mathbf{x}) = b_c, & \mathbf{x} \in \Gamma_{sc}, \\ \phi(\mathbf{x}) > b_c, & \mathbf{x} \in \Omega_s, \end{array} \right. \quad (2.8)$$

where ϕ is an implicit level set function with Lipschitz continuity embedded in a higher dimension; Ω_v , Ω_s , and Ω_c are the void region, the infill region, and the coating, respectively; Γ_{cv} is the boundary between the coating and the void region and Γ_{sc} is the boundary between the coating and the infill region; b_c is the given uniform thickness of the coating. This representation is illustrated in Fig. 2.2.

In the VFLS method, the advancement of the level set function ϕ is driven by a designable normal velocity field, which is interpolated by basis functions. There are many options for the basis functions, such as the compactly supported radial basis function (CS-RBF), the exponential function, or the Shepard function. In this paper, we use the following piece-wise function as the

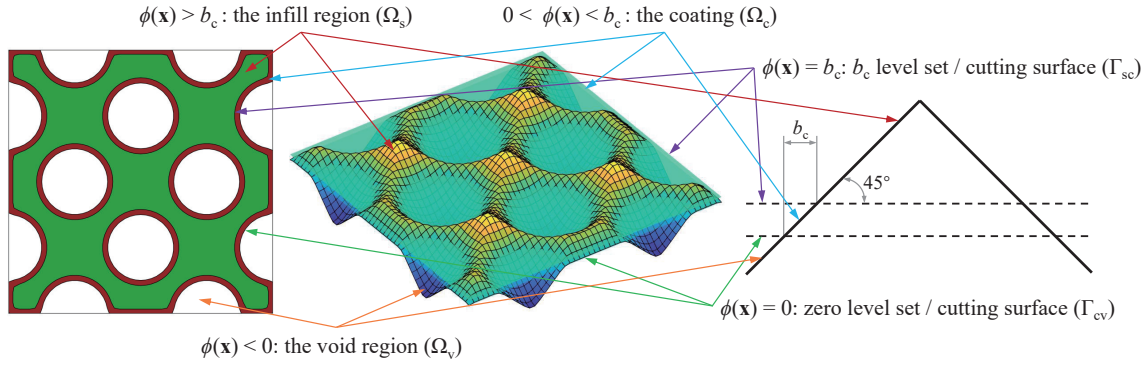


FIGURE 2.2: Illustration of a coated structure with an outer coating of uniform thickness

basis function to interpolate the design variables, which satisfies the Kronecker delta property.

$$p_j(\mathbf{x}) = \begin{cases} 1, & \|\mathbf{x} - \mathbf{x}^j\|_\infty \leq \frac{h}{2} \\ 0, & \|\mathbf{x} - \mathbf{x}^j\|_\infty > \frac{h}{2} \end{cases}, \quad j = 1, 2, \dots, N, \quad (2.9)$$

where $p_j(\mathbf{x})$ is the given basis function; N is the total number of velocity points; $\mathbf{x}^j$ is the coordinate of the j -th level set grid point and h is the size of the support domain of the basis function. In this case, the design variables are the normal velocity values $V_j^n = V^n(\mathbf{x}_j)$ defined at the level set grid points. Then, the construction of the normal velocity field can be expressed as

$$V^n(\mathbf{x}, t) = \sum_{j=1}^N V_j^n(t) p_j(\mathbf{x}), \quad j = 1, 2, \dots, N, \quad (2.10)$$

where t is the pseudo-time and $V_j^n(t)$ are the velocity design variables defined at specific points (hereafter referred to as velocity points).

After obtaining the normal velocity field $V^n(\mathbf{x}, t)$, the evolution of the topology and shape of macro design domain is governed by solving the Hamilton-Jacobi equation

$$\frac{\partial \phi}{\partial t} - V^n |\nabla \phi| = 0. \quad (2.11)$$

The signed distance property of the level set function is the key to achieve a coating with a uniform thickness. In order to preserve this important property, a re-initialization process is implemented to regulate the level set function ϕ by solving the following equation

$$\frac{\partial \phi}{\partial t} + \text{sign}(\phi_0) (|\nabla \phi| - 1) = 0, \quad (2.12)$$

where ϕ_0 is the level set function before re-initialization.

Different from many other level set-based approaches using the steepest descent method (Feynman, Allaire, Dapogny, and Jolivet, 2020; Li, Yamada, Jolivet, Furuta, Kondoh, Izui, and Nishiwaki, 2021), the construction of the normal velocity field enables the introduction of general mathematical programming algorithms (e.g., the method of moving asymptotes (MMA) (Svanberg, 1987)). Therefore, topology optimization with multiple constraints or additional design variables can be handled much easier (Wang and Kang, 2019), which is one of the advantages of the VFLS method. Besides, due to the same definition and evolution of the level set function as other conventional LSM, the VFLS method still retains the versatility of the LSM, including the signed distance property which is needed for the description of the coating with uniform thickness.

Macroscopic optimization model

Using the velocity field-based level set method, the design variables in the macroscale coated structures design are the normal velocity design variables, as follows:

$$\mathbf{V} = \{V_1^n, V_2^n, \dots, V_N^n\}^T. \quad (2.13)$$

Considering the outer coating, the elasticity matrix of a unit cell in the macroscale optimization model can be expressed by

$$\mathbf{D}^{\text{MA}} = \mathbf{D}^{\text{H}}(\boldsymbol{\eta})H(\phi - b_c) + \mathbf{D}_c(H(\phi) - H(\phi - b_c)), \quad (2.14)$$

where $H(\xi)$ is the Heaviside function, when $\xi > 0$, $H(\xi) = 1$; when $\xi < 0$, $H(\xi) = 0$. Similarly, for the macroscale material density, we have

$$\rho^{\text{MA}} = \rho^{\text{H}}(\boldsymbol{\eta})H(\phi - b_c) + \rho_c(H(\phi) - H(\phi - b_c)). \quad (2.15)$$

Compared with the density filtering-based coating model, Eqs. (2.14) and (2.15) provide an explicit relationship between the geometrical representation and material properties, respectively shown in Figs. 2.3a and b.

Remark. In this research, we select the VFLSM to deal with multiple materials at the macro scale and a more rigorous interpretation of the unit cell distribution can be yielded. Besides, it's pretty easy for us to maintain the uniform thickness of the outer coating during the optimization using the VFLSM. At the microscale, only one kind of material needs to be dealt with and we choose the SIMP method mainly because of its simplicity of numerical implementation. In addition, the VFLSM can use general optimizers (such as the MMA in this research) to perform numerical optimization and multiple constraints with two types of design variables can be handled straightforwardly. Although we use the SIMP method to conduct microscale topology optimization, there are no fundamental difficulties in using the VFLSM for the microscale topology optimization.

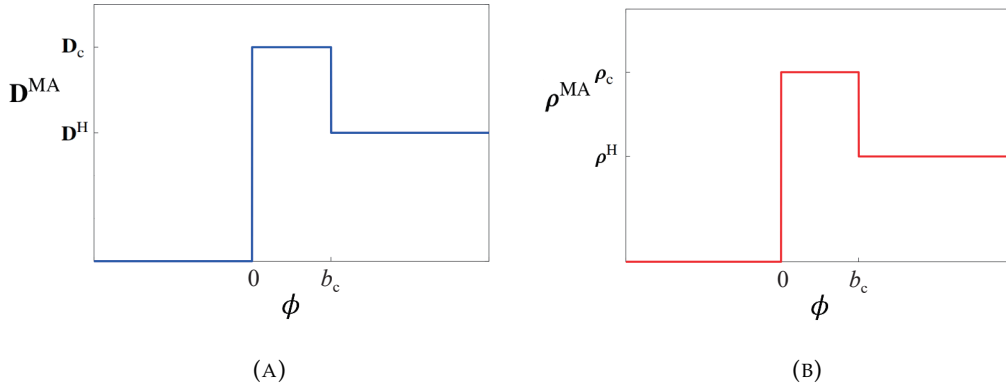


FIGURE 2.3: Illustration of the material interpolation (a) macroscale elasticity matrix expressed by Eq. (2.14); (b) macroscale material density expressed by Eq. (2.15).

2.3 Optimization problem of maximizing the fundamental eigenfrequency

Here we follow the lead of Allaire and Jouve (Allaire and Jouve, 2005) and start with the description of the eigenvalue problem in the linearized elasticity. A continuum structure occupied by an isotropic linear elastic solid material can be represented as a domain $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) with the Lipschitz continuous boundary consisted of two disjoint segments, as follows:

$$\partial\Omega = \Gamma_N \cup \Gamma_D, \quad (2.16)$$

where a Neumann boundary condition is imposed on Γ_N and a Dirichlet boundary condition on Γ_D . During optimization, it is required that all admissible designs Ω should stay in a fixed reference domain $D \subset \mathbb{R}^d$, i.e., $\Omega \subset D$.

The eigenfrequency ω and the associated eigenvector $\mathbf{u}$, i.e., the displacement field in Ω , are the solution of the following eigenvalue problem for the linear elastic system

$$\begin{cases} -\operatorname{div}(\sigma(\mathbf{u})) = \omega^2 \rho \mathbf{u} & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_D \\ \sigma(\mathbf{u})\mathbf{n} = 0 & \text{on } \Gamma_N, \end{cases} \quad (2.17)$$

where $\sigma(\mathbf{u}) = A e(\mathbf{u})$ is the stress tensor; A describes the Hooke's law; $e(\mathbf{u})$ is the strain tensor; ω is the eigenfrequency; $\mathbf{n}$ denotes the unit outward normal to the boundary.

The weak form of the undamped free vibration problem can be expressed as

$$a(\mathbf{u}, \mathbf{v}, \phi) = \lambda b(\mathbf{u}, \mathbf{v}, \phi), \quad \forall \mathbf{v} \in U, \quad (2.18)$$

where λ is the eigenvalue; $U = \{\mathbf{v} \in H^1(\Omega)^d \mid \mathbf{v} = 0 \text{ on } \Gamma_D\}$ is the space of kinematically admissible displacement fields; The energy bilinear form $a(\mathbf{u}, \mathbf{v}, \phi)$ and load linear form $b(\mathbf{u}, \mathbf{v}, \phi)$ are respectively expressed as

$$a(\mathbf{u}, \mathbf{v}, \phi) = \int_{\Omega} \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{v}) d\Omega, \quad (2.19a)$$

$$b(\mathbf{u}, \mathbf{v}, \phi) = \int_{\Omega} \rho^{\text{MA}} \mathbf{u} \mathbf{v} d\Omega. \quad (2.19b)$$

Concurrent two-scale topology optimization of coated structures with layer-wise graded microstructures infill for maximization of the fundamental eigenfrequency can be then formulated as

$$\begin{aligned} \max_{\eta, \mathbf{V}} \quad & J(\mathbf{u}, \phi) = \omega_1^2 = \lambda_1 \\ \text{s.t.} \quad & \begin{cases} a(\mathbf{u}, \mathbf{v}, \phi) = \lambda_1 b(\mathbf{u}, \mathbf{v}, \phi), \quad \forall \mathbf{v} \in U, \\ G^{\text{MA}} = \int_D H(\phi) d\Omega - f^{\text{MA}} V_D \leq 0, \\ G^{\text{MI}} = \sum_{l=1}^L \int_{\Omega_l} \left(\left(\sum_{e=1}^{n^{\text{MI}}} \eta_l^e s_l^e \right) / |Y_l| \right) H(\phi - b_c) d\Omega - f^{\text{MI}} \int_D H(\phi - b_c) d\Omega \leq 0, \\ \mathbf{0} < \boldsymbol{\eta}_{\min} \leq \mathbf{J} \leq \mathbf{1}, \quad \underline{\mathbf{V}} \leq \mathbf{V} \leq \overline{\mathbf{V}}, \end{cases} \end{aligned} \quad (2.20)$$

where f^{MA} and f^{MI} are the maximum allowed volume fractions for the macroscale and microscale, respectively; G^{MA} and G^{MI} are macroscale and microscale volume constraints used to respectively restrict the volume of macrostructure and microstructures; s refers to the volume of a microscale element.

2.4 Sensitivity analysis

2.4.1 Sensitivity analysis of simple eigenfrequency

Sensitivity analysis with respect to macroscale design variables

According to Eq. (2.20), the Lagrangian can be constructed as

$$L(\mathbf{u}, \mathbf{v}, \phi) = J(\mathbf{u}, \mathbf{v}, \phi) + a(\mathbf{u}, \mathbf{v}, \phi) - \lambda_1 b(\mathbf{u}, \mathbf{v}, \phi). \quad (2.21)$$

To consider the shape sensitivity of the objective functional J with respect to the material domain Ω , we introduce a shape perturbation $\boldsymbol{\theta}$ to the material domain Ω , yielding a perturbed domain $\Omega_{\boldsymbol{\theta}} = (\mathbf{Id} + \boldsymbol{\theta})\Omega$ (Allaire and Jouve, 2005; Wang and Kang, 2018b),

$$J((\mathbf{Id} + \boldsymbol{\theta})\Omega) = J(\Omega) + J'(\Omega)(\boldsymbol{\theta}) + o(\boldsymbol{\theta}), \quad \lim_{\|\boldsymbol{\theta}\| \rightarrow 0} \frac{|o(\boldsymbol{\theta})|}{\|\boldsymbol{\theta}\|} = 0. \quad (2.22)$$

Therefore, the shape derivative of the Lagrangian function is

$$\frac{\partial L(\mathbf{u}, \mathbf{v}, \phi)}{\partial t} = \lambda'_1 + a'(\mathbf{u}, \mathbf{v}, \phi) - \lambda_1 b'(\mathbf{u}, \mathbf{v}, \phi) - \lambda'_1 b(\mathbf{u}, \mathbf{v}, \phi), \quad (2.23)$$

where the material derivatives of $a(\mathbf{u}, \mathbf{v}, \phi)$ and $b(\mathbf{u}, \mathbf{v}, \phi)$ are respectively given by

$$\begin{aligned} a'(\mathbf{u}, \mathbf{v}, \phi) &= \int_D \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}') : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{v}) H(\phi) d\Omega \\ &\quad + \int_D \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{v}') H(\phi) d\Omega \\ &\quad + \int_{\Omega} \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{v}) \delta(\phi) |\nabla \phi| V^n d\Omega, \end{aligned} \quad (2.24a)$$

$$\begin{aligned} b'(\mathbf{u}, \mathbf{v}, \phi) &= \int_D \rho^{\text{MA}} \mathbf{u}' \mathbf{v} H(\phi) d\Omega + \int_D \rho^{\text{MA}} \mathbf{u} \mathbf{v}' H(\phi) d\Omega \\ &\quad + \int_{\Omega} \rho^{\text{MA}} \mathbf{u} \mathbf{v} \delta(\phi) |\nabla \phi| V^n d\Omega, \end{aligned} \quad (2.24b)$$

where $\mathbf{u}'$ and $\mathbf{v}'$ are the partial derivatives of $\mathbf{u}$ and $\mathbf{v}$ with respect to pseudo-time.

The adjoint equations can be derived by applying the Kuhn-Tucker condition.

$$a(\mathbf{u}', \mathbf{v}, \phi) - \lambda_1 b(\mathbf{u}', \mathbf{v}, \phi) = 0, \quad (2.25a)$$

$$a(\mathbf{u}, \mathbf{v}', \phi) - \lambda_1 b(\mathbf{u}, \mathbf{v}', \phi) = 0, \quad (2.25b)$$

$$1 - b(\mathbf{u}, \mathbf{v}, \phi) = 0. \quad (2.25c)$$

Given that the real mode $\mathbf{u}$ is the equation to the adjoint mode $\mathbf{v}$, Eq. (2.25c) is a mass-orthonormalization condition for the eigenvector. Therefore, we have

$$\begin{aligned} \frac{\partial L(\mathbf{u}, \mathbf{v}, \phi)}{\partial t} &= \lambda'_1 + \int_{\Omega} \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) \delta(\phi) |\nabla \phi| V^n d\Omega \\ &\quad - \lambda_1 \int_{\Omega} \mathbf{u} \rho^{\text{MA}} \mathbf{u} \delta(\phi) |\nabla \phi| V^n d\Omega - \lambda'_1 \end{aligned} \quad (2.26a)$$

$$= \int_{\Omega} \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) \delta(\phi) |\nabla \phi| V^n d\Omega - \lambda_1 \int_{\Omega} \mathbf{u} \rho^{\text{MA}} \mathbf{u} \delta(\phi) |\nabla \phi| V^n d\Omega. \quad (2.26b)$$

For coated structures, the material interface consists of two parts, Γ_{cv} and Γ_{sc} , and the variations of them must be considered in the derivation of the shape derivative. Thus, the sensitivity of the objective functional with respect to macroscale design variables can be expressed as

$$\frac{\partial J(\Omega_\theta)}{\partial V_j^n} = \frac{\partial J'(\Omega)(\theta)}{\partial V_j^n} \quad (2.27a)$$

$$= \int_{\Omega} \left(\boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) - \lambda_1 \mathbf{u} \boldsymbol{\rho}^{\text{MA}} \mathbf{u} \right) \delta(\phi) |\nabla \phi| p_j \, d\Omega \quad (2.27b)$$

$$= \int_{\Gamma_{\text{sc}}} \left(\left\| \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) \right\|_{\Delta} - \lambda_1 \mathbf{u} \left\| \boldsymbol{\rho}^{\text{MA}} \right\|_{\Delta} \mathbf{u} \right) p_j \, d\Gamma \quad (2.27c)$$

$$+ \int_{\Gamma_{\text{cv}}} \left(\boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}_c : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) - \lambda_1 \mathbf{u} \boldsymbol{\rho}_c \mathbf{u} \right) p_j \, d\Gamma,$$

where $\|Q(\mathbf{x})\|_{\Delta}$ is the normal-directional jump of the function $Q(\mathbf{x})$ across Γ_{sc} , i.e., $\|Q(\mathbf{x})\|_{\Delta} = Q(\mathbf{x})_{-0} - Q(\mathbf{x})_{+0}$ (Wang and Kang, 2018a).

During the concurrent two-scale topology optimization, the thickness of the coating remains unchanged under the shape perturbation θ . It should be noted that the perturbations θ on Γ_{sc} and Γ_{cv} are not independent and they have the following relationship: $(\theta \cdot \mathbf{n})(\mathbf{x}) = (\theta \cdot \mathbf{n})(P_{\Gamma_{\text{cv}}}(\mathbf{x}))$ for $\forall \mathbf{x} \in \Gamma_{\text{sc}}$, where $P_{\Gamma_{\text{cv}}}(\mathbf{x})$ is the projection point of $\mathbf{x}$ on the boundary Γ_{cv} (Allaire, Jouve, and Michailidis, 2016). Therefore, the integral on Γ_{sc} can be transformed to one on Γ_{cv} , which can simplify the sensitivity analysis. We denote the first term on the right side of the above equation as T_1 , then we have

$$T_1 = \int_{\Gamma_{\text{cv}}} g_1 |\det(\mathbf{I} - b_c \nabla \mathbf{n})| p_j \, d\Gamma = \int_{\Gamma_{\text{cv}}} g_1 \prod_{i=1}^{N'-1} (1 - b_c \kappa_i) p_j \, d\Gamma, \quad j = 1, 2, \dots, N, \quad (2.28)$$

where

$$g_1 = \begin{cases} 0, & \text{if } \mathbf{x} - b_c \mathbf{n} \notin \Gamma_{\text{sc}} \\ \left\| \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) \right\|_{\Delta} - \lambda_1 \mathbf{u} \left\| \boldsymbol{\rho}^{\text{MA}} \right\|_{\Delta} \mathbf{u} \Big|_{\mathbf{x} - b_c \mathbf{n}}, & \text{if } \mathbf{x} - b_c \mathbf{n} \in \Gamma_{\text{sc}} \end{cases}, \quad \mathbf{x} \in \Gamma_{\text{cv}}. \quad (2.29)$$

N' is the dimensionality, $\kappa_i (1 \leq i \leq N' - 1)$ are the principal curvatures. Therefore, we have

$$\frac{\partial J(\Omega_\theta)}{\partial V_j^n} = \int_{\Gamma_{\text{cv}}} \left[\boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) : \mathbf{D}_c : \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) - \lambda_1 \mathbf{u} \boldsymbol{\rho}_c \mathbf{u} + g_1 \prod_{i=1}^{N'-1} (1 - b_c \kappa_i) \right] p_j \, d\Gamma, \quad j = 1, 2, \dots, N. \quad (2.30)$$

Sensitivities of volume constraints with respect to macroscale design variables are defined as

$$\frac{\partial G^{\text{MA}}}{\partial V_j^n} = \int_D \delta(\phi_j) |\nabla \phi_j| p_j \, d\Omega, \quad j = 1, 2, \dots, N, \quad (2.31a)$$

$$\begin{aligned} \frac{\partial G^{\text{MI}}}{\partial V_j^n} &= \int_D \delta(\phi_j - b_c) |\nabla \phi_j| p_j \left(\left(\sum_{e=1}^{n^{\text{MI}}} \eta_{l,k}^e S_{l,k}^e \right) / |Y_{l,k}| \right) d\Omega \\ &\quad - f_2 \int_D \delta(\phi_j - b_c) |\nabla \phi_j| p_j \, d\Omega, \quad j = 1, 2, \dots, N. \end{aligned} \quad (2.31b)$$

Sensitivity analysis with respect to microscale design variables

Similarly, for the microscale design variable η_l^e ($e = 1, 2, \dots, n^{\text{MI}}$) in the l -th layer of the macroscale lattice infill, the sensitivity of the objective function can be derived as

$$\frac{\partial J}{\partial \eta_l^e} = \int_D \left(\boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) \cdot \frac{\partial \mathbf{D}_{ijpq}^{\text{H}}}{\partial \eta_l^e} \cdot \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}) - \lambda_1 \mathbf{u} \frac{\partial \rho^{\text{MA}}}{\partial \eta_l^e} \mathbf{u} \right) H(\phi - b_c) \, d\Omega, \quad (2.32)$$

$$l = 1, 2, \dots, L; \quad e = 1, 2, \dots, n^{\text{MI}},$$

in which the first derivative of the effective elasticity matrix can be obtained as

$$\frac{\partial \mathbf{D}_{ijpq}^{\text{H}}}{\partial \eta_l^e} = \frac{1}{|\mathbf{Y}|} \int_Y \frac{\partial \mathbf{D}_{rskt}^{\text{MI}}}{\partial \eta_l^e} \left(\varepsilon_{rs}^{0(ij)} - \varepsilon_{rs}^* \left(\chi^{ij} \right) \right) \left(\varepsilon_{kt}^{0(pq)} - \varepsilon_{kt}^* \left(\chi^{pq} \right) \right) \, d\mathbf{y} \quad (2.33a)$$

$$= \frac{1}{|\mathbf{Y}|} \int_Y \xi \left(\eta_{l,k}^e \right)^{\xi-1} (E_0 - E_{\min}) \mathbf{D}_{rskt}^0 \left(\varepsilon_{rs}^{0(ij)} - \varepsilon_{rs}^* \left(\chi^{ij} \right) \right) \left(\varepsilon_{kt}^{0(pq)} - \varepsilon_{kt}^* \left(\chi^{pq} \right) \right) \, d\mathbf{y}, \quad (2.33b)$$

$$l = 1, 2, \dots, L; \quad e = 1, 2, \dots, n^{\text{MI}}.$$

The second derivative of the macroscale material density matrix is

$$\frac{\partial \rho^{\text{MA}}}{\partial \eta_l^e} = \frac{\partial \rho^{\text{MA}}}{\partial \eta_l^e} H(\phi - b_c) = (\rho_0 - \rho_{\min}) H(\phi - b_c), \quad l = 1, 2, \dots, L; \quad e = 1, 2, \dots, n^{\text{MI}}. \quad (2.34)$$

Sensitivities of volume constraints with respect to microscale design variables can be respectively expressed as

$$\frac{\partial G^{\text{MA}}}{\partial \eta_l^e} = 0, \quad l = 1, 2, \dots, L; \quad e = 1, 2, \dots, n^{\text{MI}}, \quad (2.35a)$$

$$\frac{\partial G^{\text{MI}}}{\partial \eta_l^e} = \sum_{k=1}^{n_l^{\text{MA}}} H(\phi_{l,k} - b_c) \left(s_{l,k}^e / |Y_{l,k}| \right), \quad l = 1, 2, \dots, L; \quad e = 1, 2, \dots, n^{\text{MI}}. \quad (2.35b)$$

2.4.2 Sensitivity analysis of multiple eigenfrequencies

As a commonly encountered issue for the eigenfrequency optimization, multiple eigenfrequencies may happen showing several individual eigenmodes but with similar eigenfrequencies. Sometimes they even coincide with the considered eigenfrequency and cause serious interference between themselves. The sensitivity of multiple eigenfrequencies is not unique due to the lack of usual differentiability properties of the subspace spanned by the eigenvectors associated with multiple eigenfrequencies (Seyranian, Lund, and Olhoff, 1994). To deal with this issue, we follow the research of Xu et al. (Xu, Wang, and Xie, 2019) and use the modal assurance criterion (MAC) method (Pastor, Binda, and Harčarik, 2012). The definition of MAC is

$$\text{MAC}(\mathbf{u}_a, \mathbf{u}_b) = \frac{|\mathbf{u}_a^T \mathbf{u}_b|^2}{(\mathbf{u}_a^T \mathbf{u}_a)(\mathbf{u}_b^T \mathbf{u}_b)}, \quad (2.36)$$

where $\mathbf{u}_a$ represents the reference eigenvector of the current iteration step and $\mathbf{u}_b$ refers to the objective eigenvector of the previous iteration step. The value of the MAC is a scalar constant revealing the degree of consistency between $\mathbf{u}_a$ and $\mathbf{u}_b$, which varies from 0 (representing no consistent correspondence) to 1 (representing a consistent correspondence).

With the MAC value, a new objective eigenvector can be obtained in each iteration step by comparing a few reference eigenvectors with the objective eigenvector $\mathbf{u}_{obj}$ as

$$\mathbf{u}_{obj}^n = \mathbf{u}_\zeta^n \text{ that } \max_{\zeta} [\text{MAC}(\mathbf{u}_{obj}^{n-1}, \mathbf{u}_\zeta^n)], \quad \zeta = 1, 2, \dots, N_m, \quad (2.37)$$

where N_m is the number of reference eigenvectors. At the n -th iteration step, objective eigenvector of the previous iteration step $\mathbf{u}_{obj}^{n-1}$ is used to calculate the MAC value.

2.5 Numerical examples

In this section, several 2D numerical examples covering different layers of lattice infill and different coating thicknesses are presented to demonstrate the effectiveness of the proposed concurrent multiscale topology optimization framework. For the coating material, the Young's modulus is $E_c = 200 \text{ GPa}$ and the material density is $\rho_c = 7200 \text{ kg m}^{-3}$. For the base material of lattice infill, the Young's modulus is $E_0 = 135 \text{ GPa}$ and the material density is $\rho_0 = 5600 \text{ kg m}^{-3}$. Both materials have the same Poisson's ratio $\nu_0 = 0.3$. In all examples, different layers of the lattice infill are uniformly (or near-uniformly) distributed along a specific direction. The size of a macroscale element is set to 1 and one macroscale unit cell is discretized into 40×40 uniformly-sized planar square bilinear elements. The radius of the density filter for microstructures is $r_{\min} = 2$. After the iteration step reaches 100 and volume fractions of macrostructures and microstructures are all within the 0.5% of the required volume fractions, the iteration of multiscale topology optimization will terminate if one of the following conditions is satisfied: (1) Five previous values of the objective function differ by less than 10^{-3} . (2) The relative difference of objective function values between adjacent iterations falls below 10^{-5} .

2.5.1 Example 1: A cantilever beam

Considering different layers of lattice infill

The first example here is a cantilever beam clamped at the left edge, as shown in Fig. 2.4a. The length and the height of the structure are 0.2 m and 0.1 m, respectively. The thickness of the coating is given as $b_c = 0.0008$ m and a concentrated mass of 500 kg is imposed on the middle two macro elements of the right edge. In this example, for both macroscale and microscale, the maximum allowed upper volume fractions (f^{MA} and f^{MI}) are set to 45%.

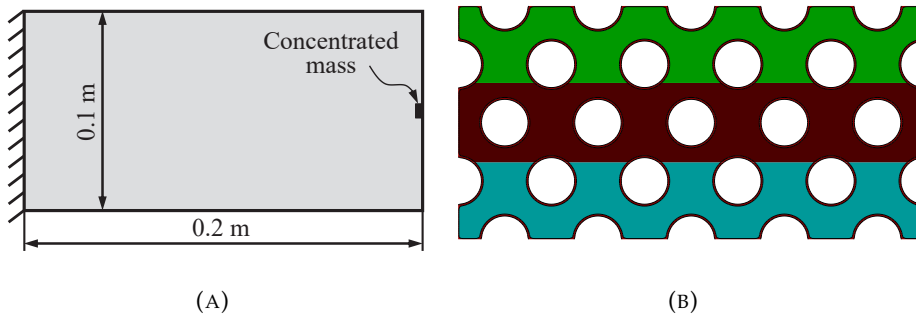


FIGURE 2.4: Structural representation of the cantilever beam (a) design domain; (b) initial macroscale design for the case of three layers.

To begin with, we consider the case of a coated cantilever beam with three uniformly-divided layers ($L=3$) of the lattice infill. The initial macroscale structural design is given in Fig. 2.4b, denoted by different colors to show different layers. After 174 steps of iteration, the final optimization results are obtained, as shown in Fig. 2.5a. As can be seen, the optimal macroscale structural topology features binary structures due to the use of the VFLS method. Besides, the uniform thickness of the coating is well-maintained. The microstructures for all the three layers are clear and reasonable. Patterns of microstructures for the top and bottom layers are symmetric to each other with respect to the central axis of the design domain. Besides, material layout for the middle layer of the lattice infill is quite different from others, which proves that considering multiple layers of the lattice infill can provide higher design flexibility and leads to various microstructural topologies.

According to the iteration history shown in Fig. 2.5b, structural volume fractions at both two scales are well converged and reach their prescribed values. Despite a significant drop at the beginning with the fast decrement of two-scale volume fractions, the fundamental eigenfrequency smoothly increases and generally stabilizes, yielding a final function value of $J = 6.13$ Hz. However, it can be seen that the final value of the fundamental eigenfrequency is smaller than that around the 50th step, which means the final structure we optimized is a local optimum. The reason for this phenomenon is the break of material members at the macro scale caused by the

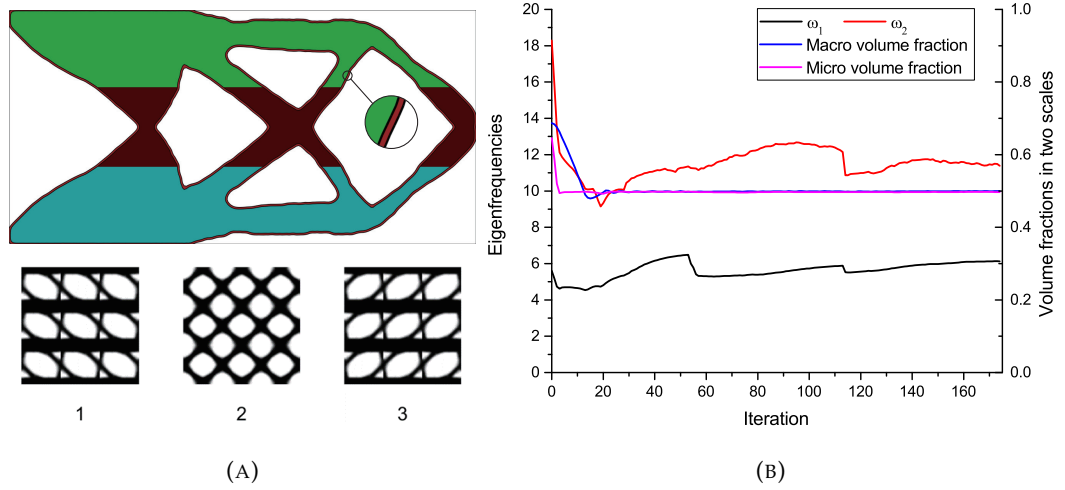


FIGURE 2.5: The cantilever beam with the coating of 0.0008 m and three-layer graded lattice infill: (a) macroscale and microscale optimization result; (b) iteration history.

macroscale volume fluctuation. To alleviate this issue, one can add a size control or reduce the bound between the minimum and maximum values of the velocity field. However, structures with high performance can still be optimized using the proposed method.

To further study the potential of layer-wise graded lattice infill for coated structures, we then consider other numbers of divided layers, including one ($L=1$, periodic and uniform microstructures), two ($L=2$), four ($L=4$), and five ($L=5$). Material properties and other design parameters are set as the same as the three-layer case. The optimal solutions for those test cases are shown in Fig. 2.6. At macroscale, structural topologies are varied from each other but all have clear boundaries with uniform coating. As can be seen, microstructural patterns for the top and bottom layers are very similar in these multi-layer cases. For coated structures with three-layer (cf. Fig. 2.5a) and four-layer (cf. Fig. 2.6c) lattice infill, microstructures for the middle region of the substrate area are almost the same. The second and the fourth layer of the coated cantilever beam with five-layer lattice infill (cf. Fig. 2.6d) are occupied by bar-like structures, which also reveals various layer division can generate novel microstructural configurations. Moreover, all parts of optimized microstructures are connectable between different layers. It should be noted that no special technique has been introduced into the proposed method to ensure the connectivity of microstructures between different layers. To guarantee the generation of well-connected microstructural configurations, additional techniques can be utilized, such as the kinematically connective constraint approach (Zhou and Li, 2008), the designable connective region method (Liu, Kang, and Luo, 2020), and the artificial post-processing of connecting regions (Li, Luo, Gao, and Walker, 2018).

The comparison of the fundamental eigenfrequency of coated cantilever beams with different layers of graded lattice infill is shown in Fig. 2.7. A clear tendency can be observed that the fundamental eigenfrequency of the cantilever beam increases when the number of divided layers grows.

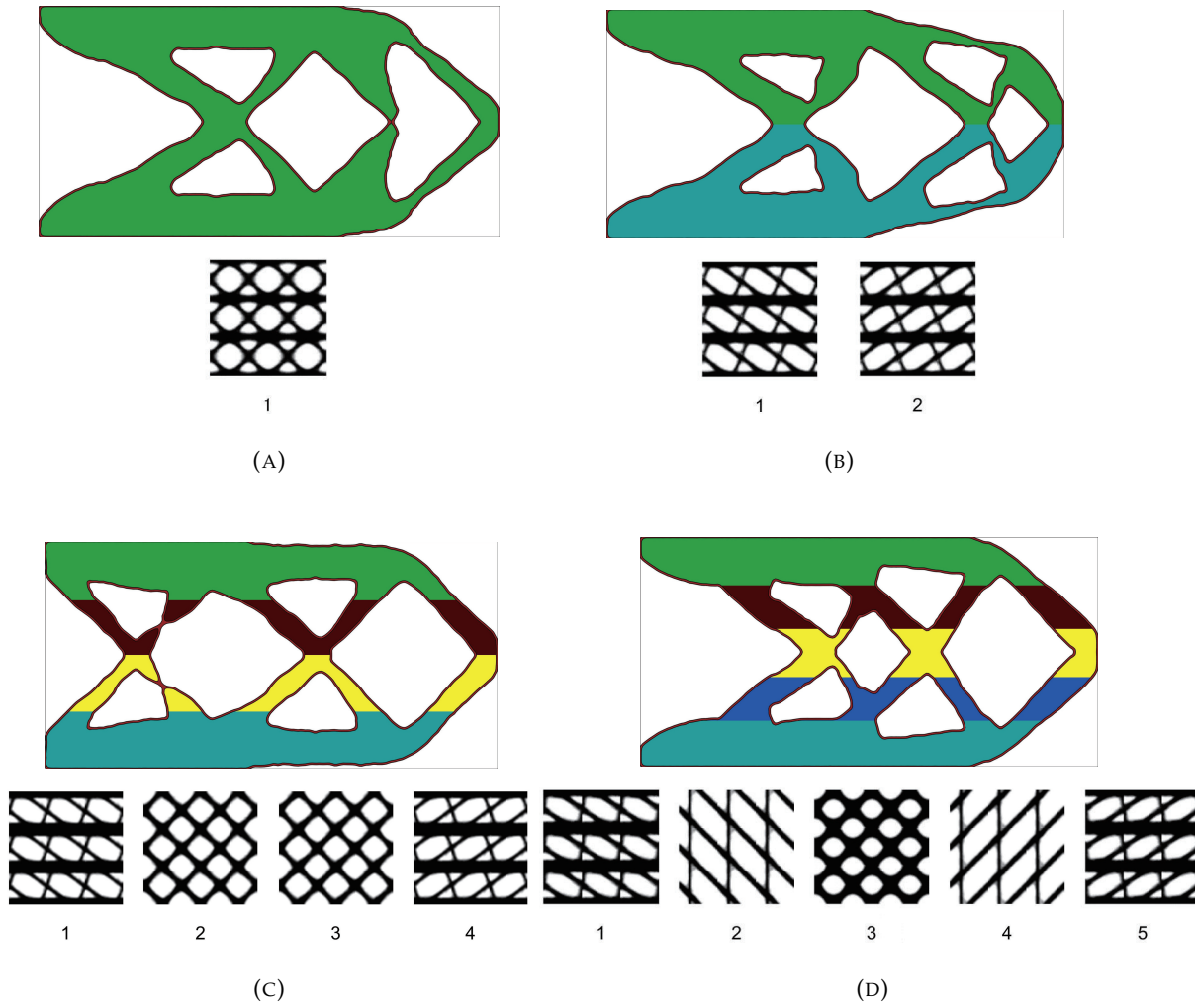


FIGURE 2.6: Macroscale and microscale optimization results of the cantilever beam with the coating of 0.0008 m: (a) periodic and uniform lattice infill; (b) two-layer graded lattice infill; (c) four-layer graded lattice infill; (d) five-layer graded lattice infill.

However, such performance improvement of the fundamental eigenfrequency becomes less significant when the number of divided layers increases, which reveals that the further increase of divided layers might have limited influence on the improvement of structural performance. In addition, the two-layer case ($\omega_1 = 5.98$ Hz) has more than 8% higher value of the fundamental eigenfrequency than the structure with periodic and uniform lattice infill ($\omega_1 = 5.51$ Hz), which proves the necessity for us to consider layer-wise graded lattice infill design.

To consider the influence of the scale ratio between different scales on the optimization results, now we reconsider the cantilever beam with periodic and uniform lattice infill ($L=1$). A different scale ratio between macrostructure and microstructure is set, i.e., 1 to 60 by 60, and optimization results are shown in Fig. 2.8. Compared to Fig. 2.6a, no obvious difference can be observed between optimization results using different scale ratios. The fundamental eigenfrequency of the structure shown in Fig. 2.8 (5.87 Hz) only has a 6.7% difference from that of the structure shown in Fig. 2.6a (5.51 Hz). It may imply that the scale ratio difference has no significant influence on the optimization results. However, a smaller scale ratio between the macrostructure and microstructure allows finer geometrical features.

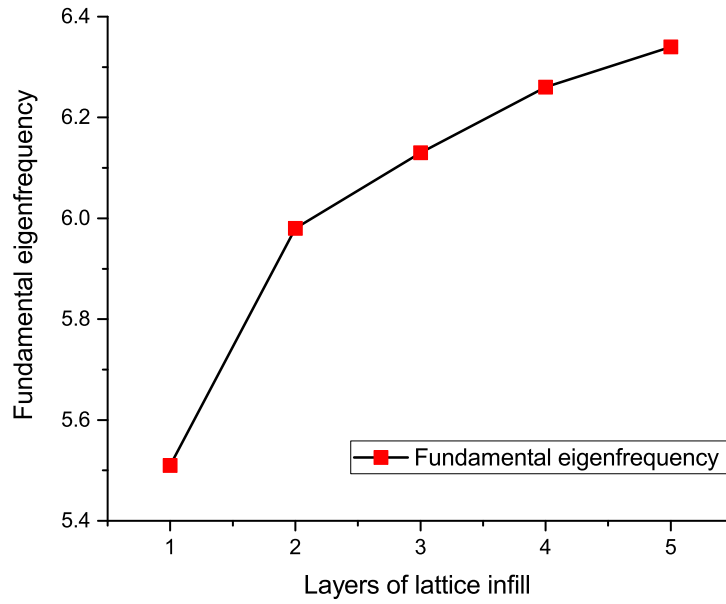


FIGURE 2.7: Comparison of the fundamental eigenfrequency of the coated cantilever beam with different layers of graded lattice infill.

Considering different coating thicknesses

In this subsection, we consider the influence of coating thickness on the optimal macroscale and microscale structural configurations. The number of layers for the graded lattice infill is set to three ($L=3$) and the thickness of the coating is redefined as $b_c = 0.0010$ m.

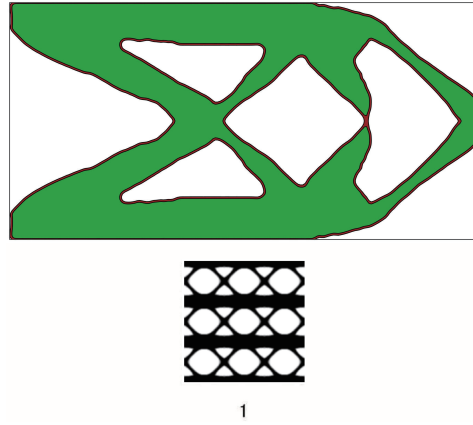


FIGURE 2.8: The cantilever beam with the coating of 0.0008 m and periodic and uniform lattice infill using the scale ratio between macrostructure and microstructure as 1 to 60 by 60.

It can be seen that the optimized macrostructure shown in Fig. 2.9a varies from the cantilever beam with the coating thickness of $b_c = 0.0008$ m (Fig. 2.5a) and more bar-like structural patterns are generated to reinforce the structure. However, the microstructural configurations for the lattice infill given in Fig. 2.9a are almost the same as the ones shown in Fig. 2.5a, which means slight difference on the coating thickness has limited influence on the microscale topologies.

The iteration history shown in Fig. 2.9b indicates great convergence. Both macroscale and microscale volume fraction constraints are satisfied. The curve of the fundamental eigenfrequency is also steady and the iteration terminates with the objective value $J = 6.28$ Hz.

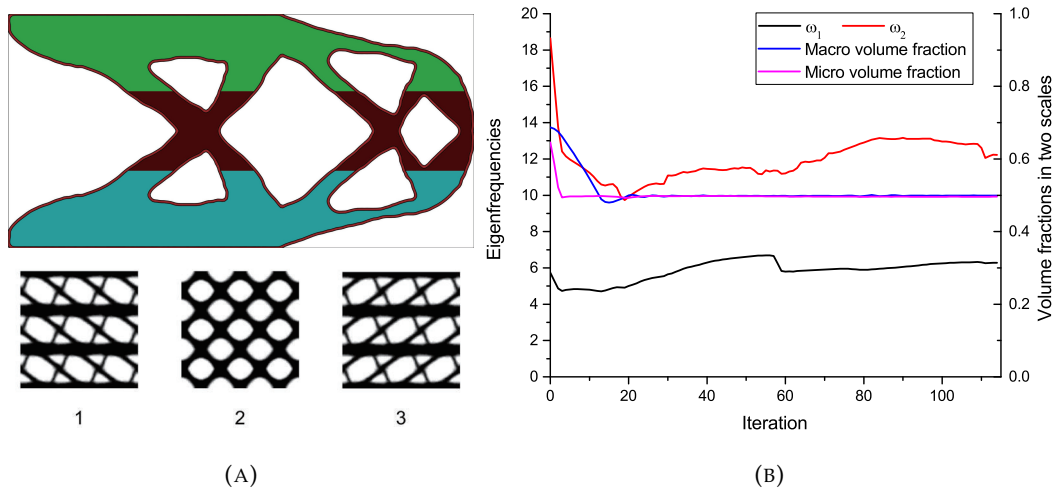


FIGURE 2.9: The cantilever beam with the coating of 0.0010 m and three-layer graded lattice infill: (a) macroscale and microscale optimization result; (b) iteration history.

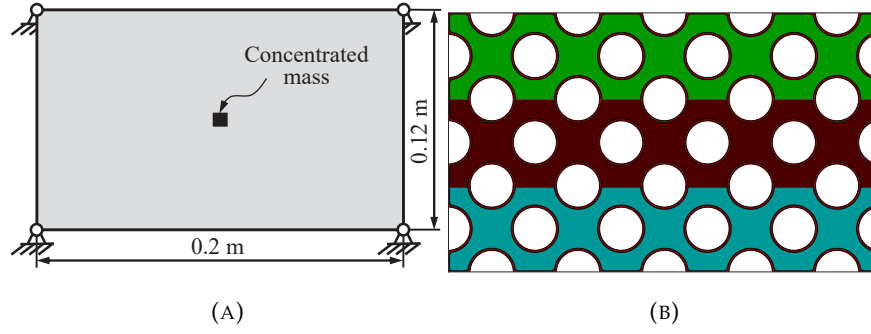


FIGURE 2.10: Structural representation of the four corner-fixed beam: (a) design domain; (b) initial macroscale design for the case of three-layer lattice infill.

2.5.2 Example 2: A four corner-fixed beam

In this example, to validate the efficiency of the introduced MAC method, we tend to make a comparison between the optimization results obtained using the MAC method and the multiplicity judgment parameter. As a popular approach to deal with multiple eigenfrequencies in the field of topology optimization, a multiplicity judgment parameter β (e.g., $\beta = 5\%$) (Hu, Ding, Shen, and Zhang, 2020; Manickarajah, Xie, and Steven, 1998) is utilized to identify the number of eigenfrequencies. Specifically, a different order of eigenfrequency is regarded as the same order as the fundamental one if their separation is less than β . For a case of Q -fold ($Q \geq 1$) eigenfrequencies, the objective value of the fundamental eigenfrequency can be modified as

$$\omega_1 = \frac{1}{Q} \sum_{g=1}^Q \omega_g, g = 1, \dots, Q. \quad (2.38)$$

With the help of the above equation, the sensitivity of multiple eigenfrequencies can be directly calculated as the case of a unimodal eigenfrequency.

The target structure is a four corner-fixed beam whose length and height are 0.2 m and 0.1 m, respectively. The thickness of the coating is set as $b_c = 0.0010$ m. As shown in Fig. 2.10a, a concentrated mass of 300 kg is added on the four macroscale elements at the central structural region. The specified macroscale upper volume fraction is $f^{\text{MA}} = 35\%$ and the microscale upper volume fraction is $f^{\text{MI}} = 45\%$.

Firstly, the periodic and uniform layout of microstructures is considered as the infill for the beam, starting from the initial macrostructure shown in Fig. 2.10b. The optimized macrostructural configurations respectively using the MAC method and the multiplicity judgment parameter β are very similar. Besides, they are all symmetric with respect to the vertical and horizontal axis of the design domain. However, the macroscale structural boundary generated using the MAC method shown in Fig. 2.11a is smooth, while the macroscale result designed with the use of the multiplicity judgment parameter β shown in Fig. 2.12a has several notches on the boundary. For

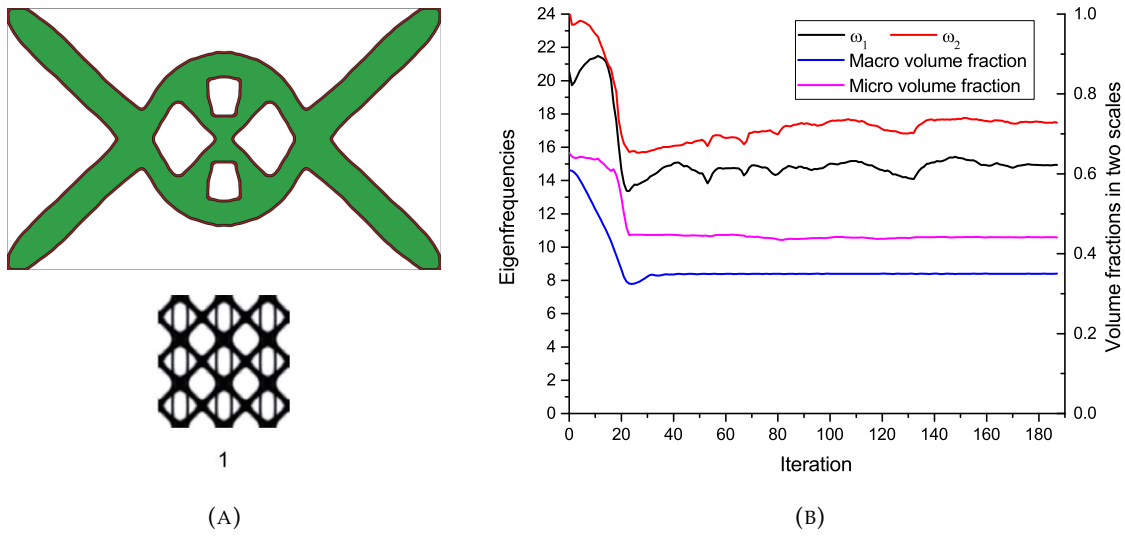


FIGURE 2.11: The four corner-fixed beam with periodic and uniform lattice infill optimized using the MAC method: (a) macroscale and microscale optimization result; (b) iteration history.

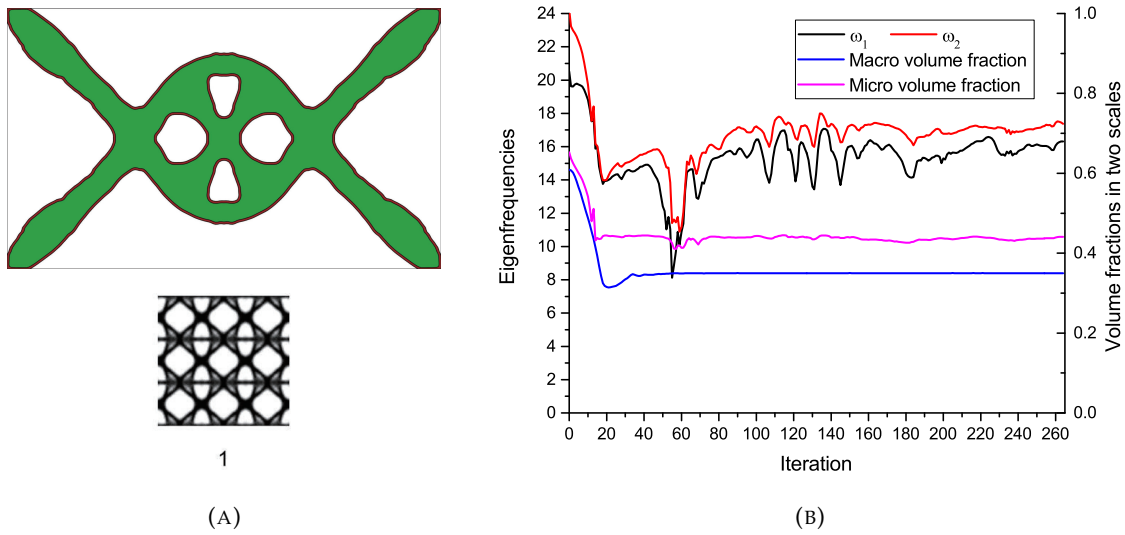


FIGURE 2.12: The four corner-fixed beam with periodic and uniform lattice infill optimized using the multiplicity judgment parameter: (a) macroscale and microscale optimization result; (b) iteration history.

the lattice infill, topologies of microstructures are clear in both cases but with different layout patterns.

It can be observed that volume fraction limits at two scales are greatly satisfied in both cases, however, the iteration curve of the fundamental eigenfrequency plotted in Fig. 2.12b has many significant ups and downs compared to the optimization history shown in Fig. 2.11b. From the view of us, the possible reason for this phenomenon is the mismatch between the fundamental eigenvector and the fundamental eigenfrequency according to Eq. (2.38). Although the structure generated using the parameter β has higher fundamental eigenfrequency value (16.31 Hz) than that shown in Fig. 2.11a (14.93 Hz), the MAC method can lead to better iteration performance and treat eigenfrequencies and their corresponding eigenvectors more accurately.

Then, we consider three-layer graded lattice infill for the four corner-fixed beam. Similarly, as the case of periodic and uniform lattice infill, the optimized macroscale structures are very similar. The symmetry of the structure is also well-maintained. At microscale, topological configurations for the top and bottom layers are also similar in these two cases. However, microstructures located at the middle layer are different between the results shown in Fig. 2.13a and Fig. 2.14a. Specifically, the concurrent topology optimization with the multiplicity judgment parameter β generates some vertical bar-form layout of material distribution at the middle region of the infill.

The volume fractions at two scales are also both satisfied in these two cases. As can be seen, the introduction of MAC method still produces great iteration history as shown in Fig. 2.13b and the optimization terminates with the final objective value $J = 17.83$ Hz. Compared to the uniform lattice infill case, there is no significant ups and downs emerge on the value of the fundamental eigenfrequency during the optimization using the parameter β , as shown in Fig. 2.14b. Despite owning a higher final fundamental eigenfrequency (17.87 Hz), the iteration curves shown in Fig. 2.13b are much smoother than those in Fig. 2.14b, which also proves the introduced MAC method shows better iteration performance than the popular multiplicity judgment parameter β .

In this numerical example, we also find that considering layer-wise graded lattice infill can further improve the eigenfrequencies of coated structures, compared to the traditional periodic and uniform lattice infill.

2.5.3 Example 3: A clamped ends beam

To further prove the efficiency of the proposed concurrent multiscale topology optimization framework, we then consider a clamped ends beam which is 0.4 m in length and 0.1 m in height, as shown in Fig. 2.15a. The thickness of the coating is $b_c = 0.0012$ m. The volume fractions at two scales are set as $f^{MA} = 45\%$ and $f^{MI} = 45\%$, respectively. A concentrated mass of 500 kg is imposed on the four macroscale elements at the central structural region and three ($L=3$) and four ($L=4$) divided layers for the graded lattice infill are considered.

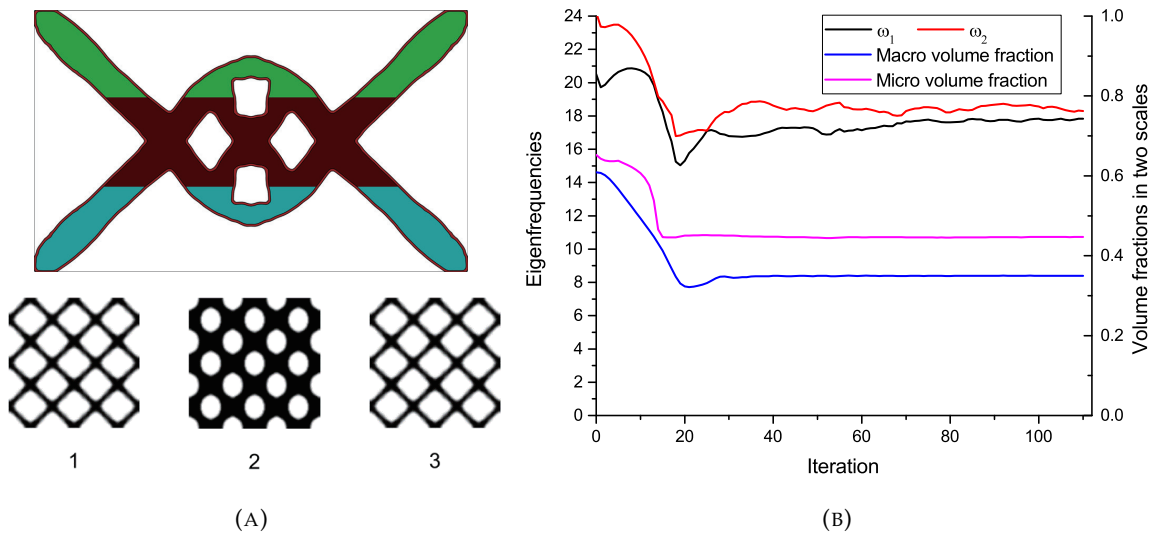


FIGURE 2.13: The four corner-fixed beam with three-layer graded lattice infill optimized using the MAC method: (a) macroscale and microscale optimization result; (b) iteration history.

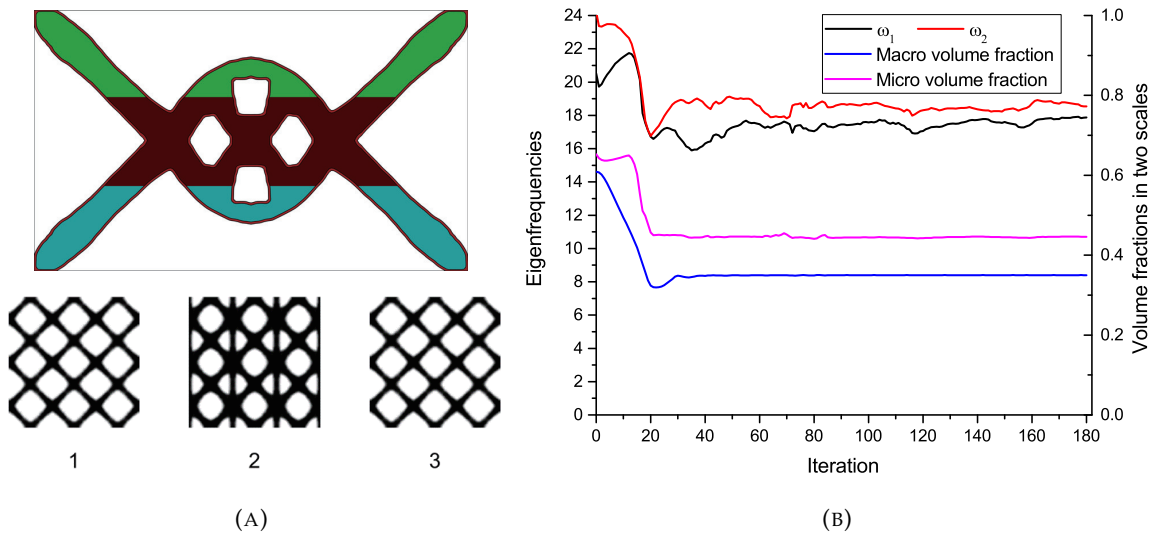


FIGURE 2.14: The four corner-fixed beam with three-layer graded lattice infill optimized using the multiplicity judgment parameter: (a) macroscale and microscale optimization result; (b) iteration history.

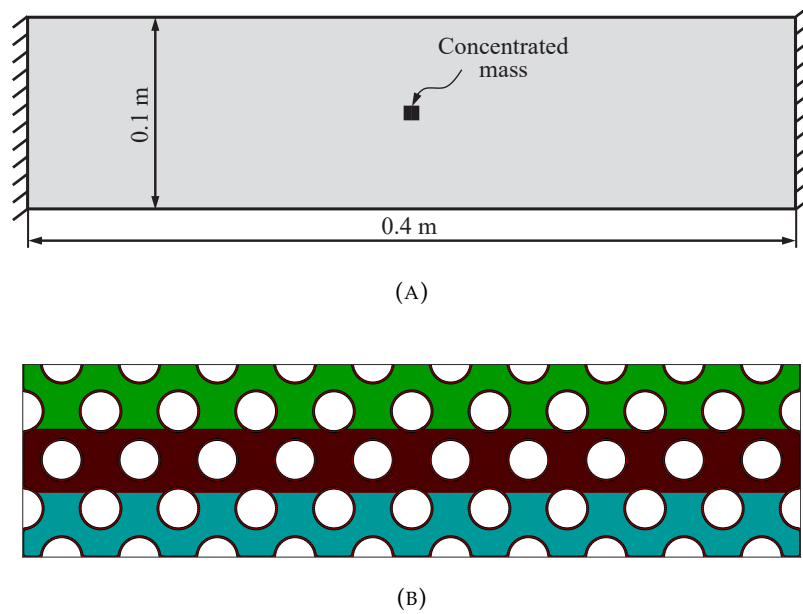


FIGURE 2.15: Structural representation of the clamped ends beam: (a) design domain; (b) initial macroscale design for the case of three-layer lattice infill.

Starting from the initial macrostructure as shown in Fig. 2.15b, the concurrent optimization results and the iteration history of the three-layer lattice infill case are given in Fig. 2.16. It can be observed that the macroscale configuration also has clear boundaries and the thickness of the coating is preserved. Patterns of the microstructures for the top and bottom layers are symmetric with each other and the microstructural topology for the middle layer is different from them. According to the curves shown in Fig. 2.16b, the fundamental eigenfrequency becomes very close to the second-order eigenfrequency when the iteration step reaches about 110, however, they remain unimodal and steady during the following optimization steps with the help of the introduced MAC method.

For the four-layer lattice infill, the optimized coated clamped ends beam is similar with the macrostructure of the three-layer case. However, from Fig. 2.17a, we observe some holes generated in the bars of the macroscale configuration. Although obtaining different results from the three-layer case, an interesting phenomenon we can see that the topologies of microstructures shown in Fig. 2.17a are very similar among different layers, which reveals that considering different layers for the lattice infill can create various optimization results. According to the iteration history plotted in Fig. 2.17b, the proposed concurrent optimization still performs great iteration performance and it terminates with the final fundamental eigenfrequency value of 10.88 Hz, which is more than 5% higher than that of the coated beam with three-layer lattice infill (10.31 Hz) and proves the potential of multi-layer graded lattice infill.

Finally, the resin-based prototypes for the generative designs with three-layer infills (cf. Fig. 2.16)

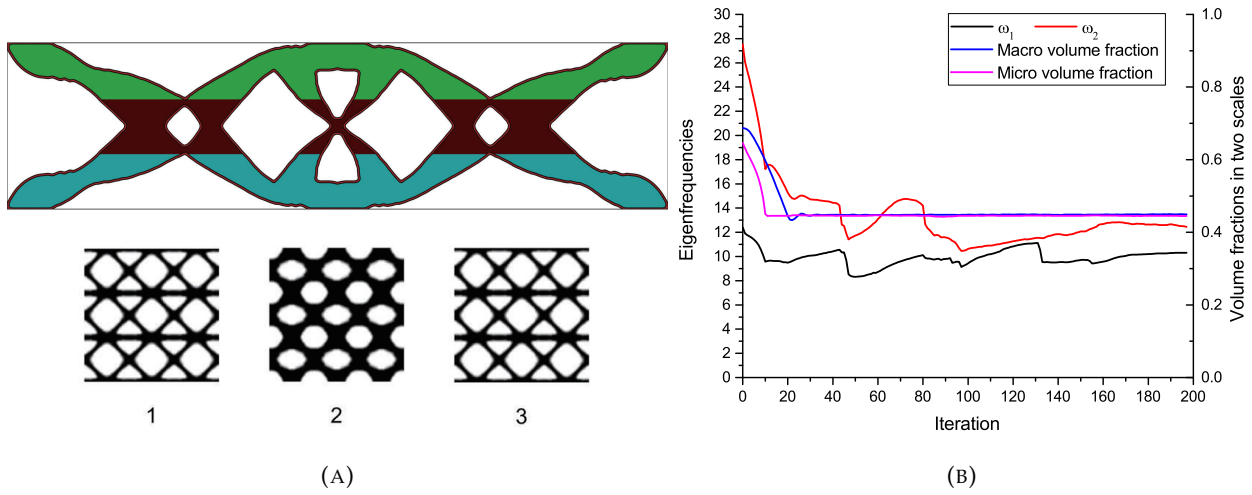


FIGURE 2.16: The clamped ends beam with the coating of 0.0012 m and three-layer graded lattice infill: (a) macroscale and microscale optimization result; (b) iteration history.

and four-layer lattice infills (cf. Fig. 2.17) are manufactured using the 3D printing. The photographs of the prototypes are respectively shown in Figs. 2.18a and b. The zoom views clearly show the details of the microstructural configurations, which confirms the manufacturability of design results using the proposed concurrent multiscale topology optimization framework.

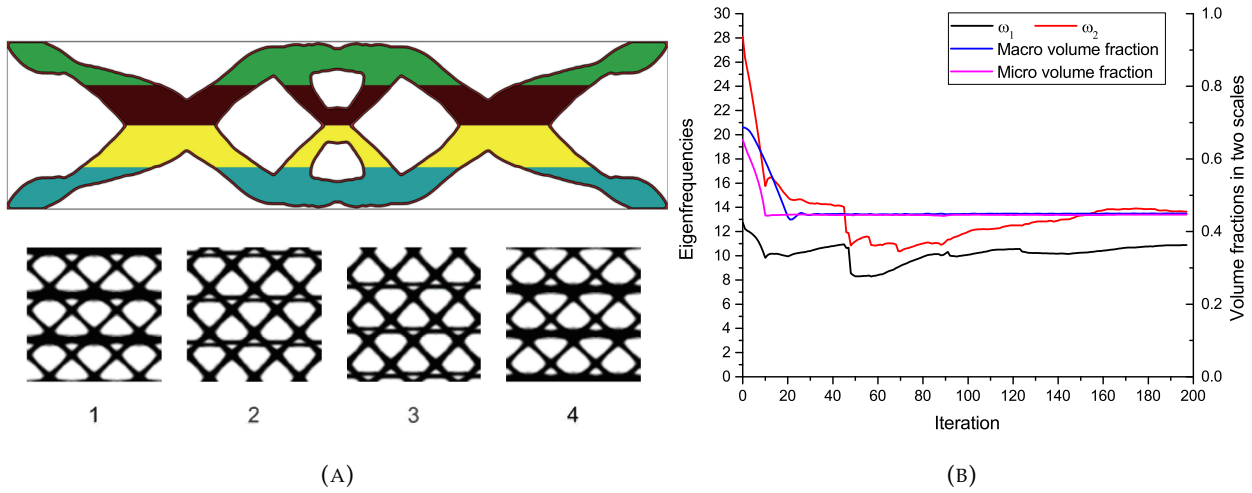


FIGURE 2.17: The clamped ends beam with the coating of 0.0012 m and four-layer graded lattice infill: (a) macroscale and microscale optimization result; (b) iteration history.

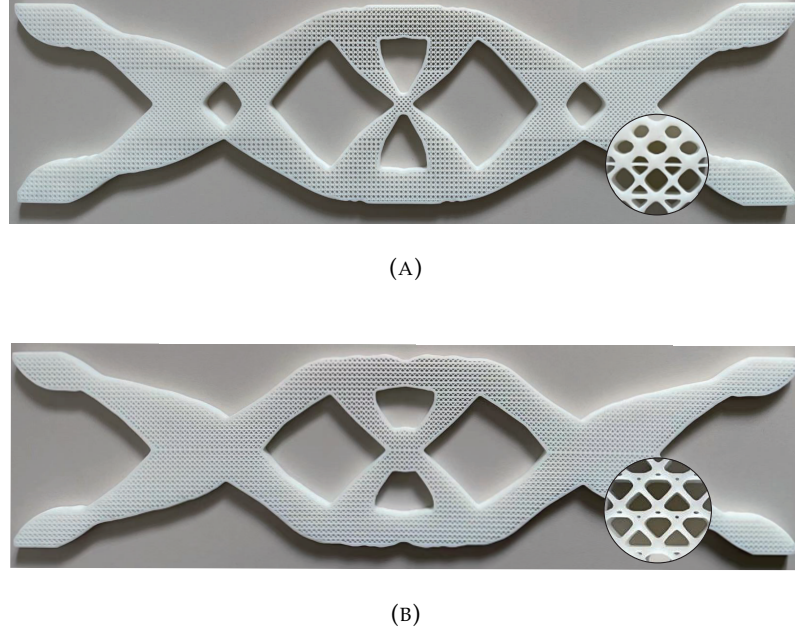


FIGURE 2.18: Manufactured coated structures with (a) three-layer and (b) four-layer graded lattice infill.

2.6 Summary

This paper studies the fundamental eigenfrequency maximization and proposes a novel concurrent multiscale topology optimization framework to design coated structures with layer-wise graded lattice infill. In this framework, the lattice infill is (near-)uniformly divided into multiple layers for various microscale material layout and covered by an outer coating of uniform thickness. The topological configuration of the macrostructure is optimized using the VFLS method to generate smooth and clear material boundaries. Due to the signed distance property, two distinct level set surfaces of only one level set function are utilized, which simplifies the description of the uniform thickness of the coating. For multi-layer lattice infill, the popular density-based method is employed to obtain different microstructural patterns. Several numerical examples show that the proposed method possesses the following remarkable features: (1) layer-wise graded lattice infill show higher fundamental eigenfrequency than those with periodic and uniform lattice infill; (2) optimized microstructures are well-connectable between neighboring layers and the generative designs can be built out using the AM technique; (3) owing to the general gradient-based algorithms, the proposed approach can handle multiple constraints efficiently; (4) compared to the popular multiplicity judgment parameter, the introduced MAC method is able to treat the fundamental eigenfrequency and its eigenvector more accurately, which leads to great iteration convergence.

Although this study only considers eigenfrequency optimization, it would be interesting to extend the proposed concurrent multiscale topology optimization framework to design coated structures with layer-wise graded lattice infill for other specific problems, such as the bone tissue scaffolds design (Wu, Fang, Entezari, Sun, Swain, Xu, Steven, and Li, [2021](#)) and buckling optimization (Thomsen, Wang, and Sigmund, [2018](#)), which are targeted in our future research.

Chapter 3

Multiscale topology optimization of coated structures for minimizing the dynamic compliance[†]

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3.1 Introduction

As commonly used in engineering, coated structures (also known as shell-infill structures) comprise an outer coating shell to cover the surface of their inner substrates for protection or for the improvement of certain functionalities. With extraordinary mechanical and physical performances (such as excellent energy absorption ability and high strength-to-weight ratio), lattice structures are ideal to be the substrate of coated structures, and this combination exhibits great potential in various fields (Tancogne-Dejean, Spierings, and Mohr, 2016; Yan, Sui, Fan, Duan, and Yu, 2020; Heimann and Lehmann, 2015), raising extensive interests in both academia and industry. In addition, from the view of additive manufacturing (AM) technology, coated structures infilled with lattice microstructural configurations are convenient to print out since inner lattice microstructures are self-supported and are able to provide support for the manufacturing of the outer coating to a large extent.

In the field of structural optimization, topology optimization owns the ability to determine the best distribution of material for concerned objectives under given constraints without prior knowledge. Over the past several decades, various topology optimization methods have been proposed, including the homogenization design (HD) method (Bendsøe and Kikuchi, 1988), the density method (Bendsøe and Sigmund, 1999), the evolutionary structural optimization (ESO)/bi-directional ESO (BESO) method (Xie and Steven, 1993; Huang, Xie, and Burry, 2006), the level set (LS)-based method (Wang, Wang, and Guo, 2003; Allaire, Jouve, and Toader, 2004), etc. Many research works have been successfully conducted on the design of coated structures using these different methods. However, varied from those density-based methods using projection, filtering, or gradient norm approaches (Yoon and Yi, 2019; Wadbro and Niu, 2019; Niu and Wadbro, 2021; Clausen, Aage, and Sigmund, 2015; Clausen, Andreassen, and Sigmund, 2017; Luo, Li, and Liu, 2019), level set methods have an unmatched advantage in the topology optimization of coated structures because they can easily describe an outer coating of uniform thickness thanks to their signed distance properties. To be specific, only two level set surfaces of one single level set function are needed for the representation of the void region, the outer coating, and the substrate area. Wang and Kang (Wang and Kang, 2018a) made use of the signed distance property of level set functions and optimized 2D and 3D coated structures. Fu et al. (Fu, Li, Gao, and Xiao, 2019) proposed a parametric LS-based topology optimization method to design shell-infill structures with periodic microstructures using the signed distance property.

Due to its great importance in engineering, topology optimization considering dynamic structural performance has attracted great attention from researchers since the pioneering research work of Díaz and Kikuchi (Díaz and Kikuchi, 1992) and has been widely studied over the past three decades. Generally, dynamic topology optimization can be divided into two categories, i.e., the maximization of eigenfrequencies and the minimum frequency response design. For the former one, Du and Olhoff (Du and Olhoff, 2007) considered simple and multiple eigenfrequencies and topologically optimized freely vibrating continuum structures. Ji et al. (Ji, Ding, and Xiong,

2014) and Li et al. (Li, Xuan, Tang, Zhu, and Yan, 2019) maximized the fundamental eigenfrequency of plate/shell structures using a biologically inspired algorithm. Based on the HD method, Y. Maeda et al. (Maeda, Nishiwaki, Izui, Yoshimura, Matsui, and Terada, 2006) developed an algorithm to design vibrating structures with desired eigenfrequencies and eigenmode shapes. Xu et al. (Xu, Wang, and Xie, 2019) proposed an isogeometric analysis (IGA)-based level set method and maximized the fundamental eigenfrequency of some typical 2D structures. Hu et al. (Hu, Ding, Shen, and Zhang, 2020; Hu, Ding, Zhang, Shen, and Li, 2023) treated the maximum fundamental eigenfrequency optimization problem and designed the stiffener layout for three-dimensional box structures. As for the frequency response minimization, Li et al. (Li, Luo, Gao, and Wu, 2018) proposed an improved parametric level set (PLS) method to minimize the frequency response of 2D and 3D structures under a given excitation frequency range, in which the Gaussian radial basis functions are used to approximate the level set functions rather than the compactly supported radial basis functions selected in conventional parametric level set methods. Zhang et al. (Zhang, Ding, Ni, Chen, Zhang, and Li, 2022) optimized a damping composite layer at two scales to achieve the minimum global frequency response (known as dynamic compliance, which will be used in the following content) of plate structures. Li et al. (Li, Yan, and Hong, 2016) extended their bionic growth algorithm to the minimization of dynamic compliance for plate structures. Shen et al. (Shen, Ding, Hu, Zhang, and Xu, 2021) reinforced box structures under harmonic excitation with stiffeners and tuned mass dampers. In the research of Olhoff and Du (Olhoff and Du, 2016), a ‘generalized incremental frequency (GIF) method’ with ‘incremental frequency (IF) technique’ is proposed to achieve continuous material distribution for structures subject to time-harmonic loads of high excitation frequencies. Takezawa et al. (Takezawa, Daifuku, Nakano, Nakagawa, Yamamoto, and Kitamura, 2016) developed a new objective function called complex dynamic compliance and minimized it during the optimization procedure to reduce the structural response peak at resonances. Liang et al. (Liang, Luo, Liu, Zhang, and Kang, 2021) proposed a prominent optimization strategy for designing the multi-electrode layout of sandwich electrorheological plates, which considers limited energy consumption under different vibration conditions to achieve best vibration control performance. Shu et al. (Shu, Wang, Fang, Ma, and Wei, 2011) treated local frequency response at specified points or surfaces of structures using the level set method. Recently, a few research works have witnessed the advances of coated structures with lattice infill for minimum dynamic compliance. For instance, Niu and Wadbro (Niu and Wadbro, 2021) simultaneously optimized the topologies of lattice infill microstructures and macroscale material layout for the vibrating coated structures. Zhang et al. (Zhang, Zhang, Ding, Gao, Xiao, and Liao, 2022) presented the minimum dynamic compliance design of sandwich structures, infilled with lattice microstructures, which are covered by two facial coatings of optimized thickness. Although reasonable structures at two scales can be achieved, only periodic and uniform microstructures are considered in their research.

Contrary to those optimized in most of the existing research works, coated structures found in the natural world are usually embedded with spatially-varied and non-uniform infilling, such as

the spongy and an-isotropic trabecular tissues in bones which can better adapt to the outer environmental stimuli. Recently, many research works have been presented to achieve non-periodic infilling. Groen et al. (Groen, Wu, and Sigmund, 2019) presented a two-fold topology optimization method for 2D coated structures, in which the configuration of a coated structure with orthotropic infill material was firstly optimized using a relatively coarse mesh and then projected on a fine but realizable scale to achieve non-uniform infill structures. Inspired by the structural characteristic of trabecular bones, Wu et al. (Wu, Aage, Westermann, and Sigmund, 2017) designed porous bone-like structures as the infill for given prototypes by imposing multi-regional volume constraints. Zhang et al. (Zhang, Toman, Yu, Biyikli, Kirca, Chmielus, and To, 2015) established a topology optimization method to design non-uniform hexagonal lattice structures. Chu et al. (Chu, Gao, Xiao, and Zhang, 2020) predefined several volume fractions for controllable kinds of microstructures and thus presented the topological design of coated structures infilled with multifarious microstructures. Wu et al. (Wu, Wang, Zhang, and Westermann, 2016) proposed a novel approach for achieving non-uniform infill structural design, and the manufacturability for AM was ensured using rhombic lattice cells. In the work of Han and Lu (Han and Lu, 2018), a size gradient method (SGM) was developed for the non-uniform lattice structural design by optimizing the geometrical size and distribution of unit cells. Lee et al. (Lee, Kwon, Yoo, Min, Nomura, and Dede, 2021) investigated multiscale topology optimization of coated structures embedded with spatially-varying orthotropic infill material, using a de-homogenization scheme that combined explicit geometrical representation with a projection method. Another effective and popular way to achieve inhomogeneous material properties is to design lattice structures consisting of multiple layers of different repetitive microstructures. Zhang et al. (Zhang, Wang, and Kang, 2019) proposed a concurrent multiscale topology optimization method for structures composed of multi-layer graded lattice microstructural configurations. Hu et al. (Hu, Wang, Zhang, Li, Ding, Izui, and Nishiwaki, 2022) studied coated structures infilled with layer-wise graded lattice structures for maximum fundamental eigenfrequency design. Li et al. (Li, Luo, Gao, and Walker, 2018) designed composites composed of multiple layers of repetitive microstructures for static and auxetic graded properties. Compared to other methods, dividing the infilling area into several layers and optimize varied microstructural configurations for certain layers is comparatively easier to achieve the inhomogeneous material properties for the infilling. Besides, such a bio-inspired design can generate functionally-graded material properties for certain considerations (Zhang, Wang, and Kang, 2019). More importantly, optimizing coated structures infilled with layer-wise microstructures achieves a trade-off balance between the structural performance and the computational cost of the optimized results. Therefore, this novel strategy is selected in this research.

Recently, another topic of great interest in the topology optimization field is to apply two or more materials to the design of structures at different scales. With multiple materials, structures may exhibit combined functionalities and own better structural performance than those made of a single material (Wang, Luo, and Yan, 2022; Wang, Luo, and Yan, 2022). In the research of Gao et al. (Gao, Luo, Li, Li, and Gao, 2019), structures composed of multi-regional material microstructures

are designed with minimization of dynamic compliance. Xu et al. (Xu, Jiang, and Xie, 2015) proposed a concurrent multiscale optimization method to design composite macrostructures and bi-material microstructures. Li et al. (Li, Luo, Xiao, Gao, and Gao, 2019) developed a multiscale design framework using a parametric color level set method, and microstructures composed of multiple materials are generated for better structural performance. One great advantage of those microstructures infilled with multiple materials is that we do not need to consider the connectivity issue between different topologies of microstructures since the materials are well-connected with each other.

In the presented study, we develop a novel concurrent multiscale topology optimization framework to design coated structures infilled with layer-wise bi-material lattice infill for minimum dynamic compliance. With a combination of the velocity field-based level set (VFLS) method and the solid isotropic material with penalization (SIMP) method, the material layout of macrostructures with an outer coating of uniform thickness and the topologies of bi-material lattice infill structures are optimized simultaneously. At the macroscale, the signed distance property of the VFLS method is utilized for the structural representation, and the thickness of the coating can be well maintained. Besides, smooth macrostructural boundaries can be obtained. At the microscale, each layer of lattice microstructures is created by a periodic distribution of optimized microstructural topologies under a global microscale volume constraint. Sensitivities for the dynamic compliance minimization problem and for the static and volume constraints at different scales are derived. The influences of the number of divided layers, excitation frequency, thickness of the outer coating, damping coefficients, mesh at different scales, static constraint, as well as the division direction for the infilled layer-wise microstructural configurations are discussed through several numerical examples.

The material of this paper is arranged as follows: Section 3.2 introduces the general formulation for the dynamic compliance analysis. Section 3.3 deals with the topology optimization models at two different scales. In Section 3.4, sensitivity analysis for the dynamic compliance with respect to the design variables at two scales, i.e., macro and micro scales, is performed for the concurrent topology optimization of coated structures. Several numerical examples are presented in Section 3.5 to prove the effectiveness of the proposed method. Finally, Section 3.6 concludes the paper.

3.2 Formulations for the dynamic compliance analysis

Considering the steady-state response of a viscously damped structure with the external harmonic force at the excitation frequency ω , the vibration analysis of the structure using a level set representation can be expressed by the following equilibrium equation in the weak form (Kim, Dong, Choi, Vlahopoulos, Ma, Castanier, and Pierre, 2003; Maeda, Nishiwaki, Izui, Yoshimura, Matsui, and Terada, 2006; Nishiwaki, Saitou, Min, and Kikuchi, 2000):

$$\int_{D^{\text{MA}}} \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}(\mathbf{v}) H(\phi) d\Omega - \omega^2 \int_{D^{\text{MA}}} \mathbf{u} \boldsymbol{\rho}^{\text{MA}} \mathbf{v} H(\phi) d\Omega + i\omega \int_{D^{\text{MA}}} \mathbf{u} \mathbf{c}^{\text{MA}} \mathbf{v} H(\phi) d\Omega = l(\mathbf{v}, \phi) \quad \forall \mathbf{v} \in U, \quad (3.1)$$

where D^{MA} is the macroscale design domain, which is composed of the void area, the coating, and the substrate region for the design of a coated structure. $\boldsymbol{\varepsilon}$ is the structural strain, $\mathbf{D}^{\text{MA}}$ is the macroscale elasticity tensor, $H(\gamma)$ is the Heaviside function, which equals 1 when $\gamma > 0$ and equals 0 when $\gamma < 0$. $\boldsymbol{\rho}^{\text{MA}}$ is the macroscale density, ϕ is the level set function. $i = \sqrt{-1}$, $\mathbf{c}^{\text{MA}}$ is the viscous damping factor, $\mathbf{u}$ is the macroscale displacement field, $\mathbf{v}$ is a kinematically admissible virtual displacement and $U = \{\mathbf{u} : u_i \in H^1(\Omega), \mathbf{u} = \mathbf{u}_0 \text{ on } \Gamma_D\}$, Γ_D denotes the Dirichlet boundary, l is the load semilinear form (Ohayon and Soize, 1997) and can be expressed as

$$l(\mathbf{v}, \phi) = \int_{D^{\text{MA}}} \tilde{\mathbf{p}} \mathbf{v} H(\phi) d\Omega + \int_{D^{\text{MA}}} \mathbf{g} \mathbf{v} \delta(\phi) |\nabla \phi| d\Omega, \quad (3.2)$$

where $\tilde{\mathbf{p}}$ is the body force, $\mathbf{g}$ is the boundary traction, and $\delta(\phi)$ is the Dirac delta function.

Using the Rayleigh damping assumption (Ma, Kikuchi, and Hagiwara, 1993), the following proportional damping model is used

$$\int_{D^{\text{MA}}} \mathbf{u} \mathbf{c}^{\text{MA}} \mathbf{v} H(\phi) d\Omega = \mathcal{A} \int_{D^{\text{MA}}} \mathbf{u} \boldsymbol{\rho}^{\text{MA}} \mathbf{v} H(\phi) d\Omega + \mathcal{B} \int_{D^{\text{MA}}} \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}(\mathbf{v}) H(\phi) d\Omega, \quad (3.3)$$

where $\mathcal{A}$ and $\mathcal{B}$ are the mass-proportional damping coefficient and the stiffness-proportional damping coefficient, respectively.

Therefore, the left side of Eq. (3.1) can be rewritten as

$$a(\mathbf{u}, \mathbf{v}, \phi) = \int_{D^{\text{MA}}} (1 + i\omega \mathcal{B}) \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}(\mathbf{v}) H(\phi) d\Omega + \int_{D^{\text{MA}}} (i\omega \mathcal{A} - \omega^2) \mathbf{u} \boldsymbol{\rho}^{\text{MA}} \mathbf{v} H(\phi) d\Omega. \quad (3.4)$$

Describing the frequency response performance over the whole structure, the dynamic compliance of a coated structure can be formulated as

$$J_u = \int_{D^{\text{MA}}} \mathbf{f} \mathbf{u} H(\phi) d\Omega, \quad (3.5)$$

where $\mathbf{f}$ is the external dynamic load.

However, due to the complex form of the functional J_u , its magnitude $|J_u|$ is used to calculate the dynamic compliance, which can be formulated as

$$J_d = |J_u| = \sqrt{[\text{real}(J_u)]^2 + [\text{imag}(J_u)]^2}, \quad (3.6)$$

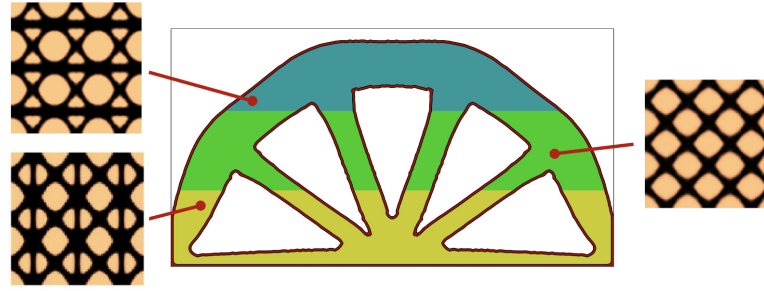


FIGURE 3.1: Illustration of a coated structure infilled with layer-wise bi-material lattice microstructures

where $\text{real}(\cdot)$ and $\text{imag}(\cdot)$ respectively refer to the real part and the image part of the “ $\cdot$ ”.

3.3 Multiscale topology optimization model

The configuration of a coated structure infilled with layer-wise bi-material lattice infill is shown in Fig. 3.1 to illustrate the novel structure we plan to design. As can be seen, the macrostructure of the coated structure is covered by an outer coating of uniform thickness, which is marked in red. The substrate area of the coated structure is uniformly divided into three layers, which are presented in different colors. Each layer of the substrate is composed of the periodic distribution of a certain type of microstructure. At the microscale, microstructural configurations are shown in a 3-by-3 repetition form and are all made of two different materials. In all examples of this research work, the black regions of the microstructures signify the microscale base material 1 and the domains in copper color are filled with the microscale base material 2.

3.3.1 Macroscale topology optimization

Macrostructural representation and the VFLS method

As a level set method, the material distribution in the VFLS method is described using an implicit level set function with Lipschitz continuity. For a coated structure with a uniform outer coating, only two level set surfaces of one single level set function are needed for the structural representation with the help of the signed distanced property (Wang and Kang, 2018a):

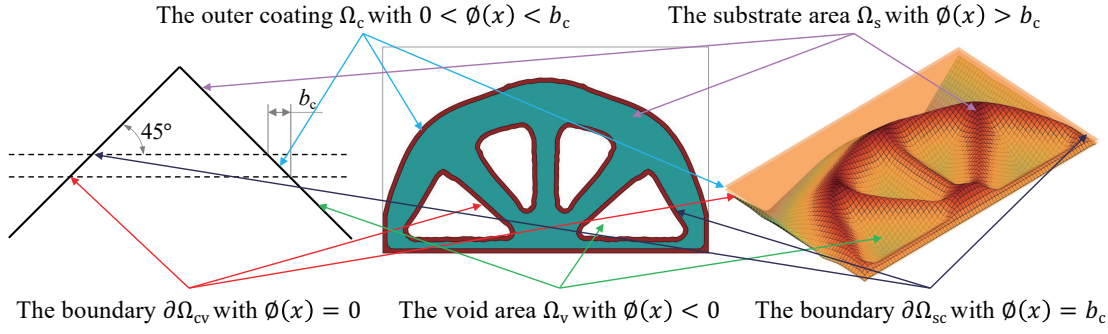


FIGURE 3.2: Illustration of a coated structure with an outer coating of uniform thickness

$$\begin{cases} \phi(\mathbf{x}) < 0, & \mathbf{x} \in \Omega_v, \\ \phi(\mathbf{x}) = 0, & \mathbf{x} \in \partial\Omega_{cv}, \\ 0 < \phi(\mathbf{x}) < b_c, & \mathbf{x} \in \Omega_c, \\ \phi(\mathbf{x}) = b_c, & \mathbf{x} \in \partial\Omega_{sc}, \\ \phi(\mathbf{x}) > b_c, & \mathbf{x} \in \Omega_s, \end{cases} \quad (3.7)$$

where ϕ is the implicit level set function. Ω_v , Ω_c , and Ω_s represent the void region, the outer coating, and the infill region, respectively. $\partial\Omega_{cv}$ is the structural boundary between the void region Ω_v and the coating Ω_c . $\partial\Omega_{sc}$ is the structural boundary between the infill region Ω_s and the outer coating Ω_c . b_c is the given thickness of the coating.

Fig. 3.2 is given here for a better illustration of the macrostructural representation for coated structures using the level set function with signed distance properties.

Using the VFLS method, the advancement of the material boundary is achieved by solving the following Hamilton-Jacobi equation with the normal boundary velocity field V^n :

$$\frac{\partial \phi}{\partial t} - V^n |\nabla \phi| = 0. \quad (3.8)$$

During the structural evolution, the signed distanced property of the level set function ϕ must be well maintained for the description of the outer coating with uniform thickness. To preserve this important property, a re-initialization process is usually implemented by using the following equation:

$$\frac{\partial \phi}{\partial t} + \text{sign}(\phi_0) (|\nabla \phi| - 1) = 0, \quad (3.9)$$

where t is the pseudo-time, and ϕ_0 is the level set function before the re-initialization treatment.

Instead of using the steepest descent method like many other level set methods (Allaire, Jouve, and Toader, 2004; Wang, Wang, and Guo, 2003), the level set function in the VFLS method is driven

by an optimized normal velocity field V^n which is interpolated by basis functions. Many different basis functions can be selected, such as the exponential function, the Shepard function, the spline basis function, etc. These functions all enable the velocity field V^n to be directly bounded between the specified minimum and maximum values of design variables, i.e., $\underline{V}^n$ and $\bar{V}^n$, and thus the CFL condition can be conveniently satisfied. In this study, the following piece-wise function that satisfies the Kronecker delta property is chosen to interpolate macroscale design variables.

$$p_j(\mathbf{x}) = \begin{cases} 1, & \|\mathbf{x} - \mathbf{x}^j\|_\infty \leq \frac{h}{2} \\ 0, & \|\mathbf{x} - \mathbf{x}^j\|_\infty > \frac{h}{2} \end{cases} \quad j = 1, 2, \dots, N, \quad (3.10)$$

where p_j is the given basis function, $\mathbf{x}^j$ is the coordinate of the j -th level set grid point, N denotes the total number of design variable points (hereinafter named as velocity knots), and h is the size of the support domain of the basis function for the concerned velocity knot. One important property of using the selected piece-wise function is that the velocity knots are positioned at the centers of the finite elements. Then, the designable normal velocity field can be constructed as

$$V^n(\mathbf{x}, t) = \sum_{j=1}^N V_j^n(\mathbf{x}, t) p_j(\mathbf{x}), \quad j = 1, 2, \dots, N, \quad (3.11)$$

where V_j^n is the velocity design variable defined at velocity knots.

For more details about the VFLS method, readers can refer to the publication of one of the authors (Wang and Kang, 2018b; Wang and Kang, 2021).

Macroscale optimization model

In the proposed concurrent multiscale topology optimization framework, the VFLS method is selected to perform macroscale topology optimization and find the ideal material distribution of coated structures. The velocity design variables can be written in the following single vector:

$$\mathbf{V}^n = \{V_1^n, V_2^n, \dots, V_N^n\}^T \quad (3.12)$$

The macroscale material properties of the coated structure are determined by the effective material properties of the lattice infill, which are evaluated in the microscale model, and those of the coating. Therefore, the expression for the elasticity tensor of a unit cell at the macroscale level can be given as

$$\mathbf{D}^{\text{MA}} = \mathbf{D}^{\text{H}}(\eta) H(\phi - b_c) + \mathbf{D}_c (H(\phi) - H(\phi - b_c)), \quad (3.13)$$

where $\mathbf{D}^{\text{H}}$ is the homogenized elasticity tensor, and $\mathbf{D}_c$ is the elasticity tensor of the coating.

Similarly, the macroscale material density can be calculated by

$$\rho^{\text{MA}} = \rho^{\text{H}}(\eta)H(\phi - b_c) + \rho_c(H(\phi) - H(\phi - b_c)), \quad (3.14)$$

where ρ_c is the material density of the outer coating, and ρ^{H} is the homogenized material density, which is also the averaged density value over the unit cell.

3.3.2 Microscale topology optimization

Due to the great numerical simplicity, the popular SIMP method is selected to conduct microscale topology optimization to design bi-material lattice microstructural configurations. The microscale design variables are the densities of elements and expressed using η . In the SIMP method for a bi-material lattice structure, $\eta = 1$ indicates a microscale element filled with one material and $\eta = 0$ denotes that composed of the other kind of material. Considering the layer-wise lattice infill microstructures, the design variables within a unit cell k of a certain layer l at the macroscale can be described as

$$\eta_{l,k} = \left\{ \eta_{l,k}^1, \eta_{l,k}^2, \dots, \eta_{l,k}^{n_l^{\text{MI}}} \right\}^T, \quad l = 1, 2, \dots, L; \quad k = 1, 2, \dots, n_l^{\text{MA}}, \quad (3.15)$$

where n^{MI} is the total number of microscale elements within an unit cell, L is the number of divided layers for the substrate region, and n_l^{MA} is the total number of unit cells discretized within the l -th layer. Similarly, the design variables for the microscale topology optimization can be written in a single vector form as

$$\eta = \left\{ \eta_{1,1}^T, \dots, \eta_{1,n_1^{\text{MA}}}^T, \eta_{2,1}^T, \dots, \eta_{2,n_2^{\text{MA}}}^T, \dots, \eta_{L,1}^T, \dots, \eta_{L,n_L^{\text{MA}}}^T \right\}^T. \quad (3.16)$$

To bridge macroscale and microscale designs, the effective elasticity tensor of a unit cell in this study is evaluated using the energy-based homogenization method (Xia and Breitkopf, 2015). Different from the asymptotic homogenization approach (Hassani and Hinton, 1998), the energy-based method adopts average stress and strain theorems and directly applies the test unit strains (i.e., $(0, 0, 1)^T$, $(0, 1, 0)^T$, and $(0, 0, 1)^T$ in the 2D scenario) on the boundaries of the unit cell.

$$\mathbf{D}_{ijkl}^{\text{H}} = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} \mathbf{D}_{pqrs} \epsilon_{pq}^{A(\tilde{i}\tilde{j})} \epsilon_{rs}^{A(\tilde{k}\tilde{l})} d\mathbf{y}, \quad (3.17)$$

where $|\mathbf{Y}|$ is the volume of a macroscale unit cell, $\epsilon_{rs}^{A(\tilde{k}\tilde{l})}$ corresponds to the superimposed strain fields $(\epsilon_{rs}^{0(\tilde{k}\tilde{l})} - \epsilon_{rs}^{*(\tilde{k}\tilde{l})})$. $\epsilon_{rs}^{0(\tilde{k}\tilde{l})}$ corresponds to the three (2D) and six (3D) linearly independent unit test strain fields, and $\epsilon_{rs}^{*(\tilde{k}\tilde{l})}$ is the periodic fluctuation strain field. Using the Einstein index summation notation, $\epsilon_{rs}^{*(\tilde{k}\tilde{l})}$ is the $\mathbf{Y}$ -periodic solution of the following equation:

$$\int_{\mathbf{Y}} \mathbf{D}_{\tilde{i}\tilde{j}pq} \epsilon_{pq}^{*(kl)} \frac{\partial \tilde{\sigma}_{\tilde{i}}}{\partial y_{\tilde{j}}} d\mathbf{y} = \int_{\mathbf{Y}} \mathbf{D}_{\tilde{i}\tilde{j}pq} \epsilon_{pq}^{0(kl)} \frac{\partial \tilde{\sigma}_{\tilde{i}}}{\partial y_{\tilde{j}}} d\mathbf{y}, \quad (3.18)$$

where $\tilde{v}$ is the Y -periodic admissible displacement field. Readers can refer to the research work of Xia et al. (Xia and Breitkopf, 2015) for the details of the energy-based homogenization approach and its MATLAB implementation.

The elasticity tensor and material density of the elements at the microscale can be respectively constructed as

$$\mathbf{D}^{\text{MI}} = \eta^\zeta \cdot \mathbf{D}_1 + (1 - \eta^\zeta) \cdot \mathbf{D}_2, \quad (3.19)$$

where $\mathbf{D}_1$ and $\mathbf{D}_2$ are the elasticity tensors of the material 1 and material 2 for the bi-material lattice microstructures, respectively. ζ is the penalization parameter, which is usually given as not smaller than 3 (Bendsøe and Sigmund, 1999) and is set as 4 in this research.

$$\rho^{\text{MI}} = \eta \cdot \rho_1 + (1 - \eta) \cdot \rho_2. \quad (3.20)$$

where ρ_1 and ρ_2 are the material densities of the material 1 and material 2 for the bi-material lattice microstructures, respectively.

3.3.3 Concurrent multiscale topology optimization

To fully consider the interaction of structural evolution at macro and micro scales, the design variables at two different scales are ideally to be updated simultaneously. Thanks to the ability of implementing the general mathematical programming algorithms, the VFSL method introduced in the proposed approach enables a concurrent multiscale topology optimization coupled with the density method. To limit the corresponding material consumption, two volume constraints are imposed on different scales, shown as the following equations:

$$G^{\text{MA}} = \int_{D^{\text{MA}}} H(\phi) d\Omega - f^{\text{MA}} \int_{D^{\text{MA}}} d\Omega \leq 0, \quad (3.21a)$$

$$G^{\text{MI}} = \sum_{l=1}^L \int_{D_l^{\text{MA}}} \left[\left(\sum_{e=1}^{n^{\text{MI}}} \eta_l^e s_l^e \right) / |\mathbf{Y}_l| \right] H(\phi - b_c) d\Omega - f^{\text{MI}} \int_{D^{\text{MA}}} H(\phi - b_c) d\Omega \leq 0, \quad (3.21b)$$

where G^{MA} and G^{MI} are volume constraints for the macroscale and microscale material distribution, respectively. f^{MA} and f^{MI} are the given maximum macroscale and microscale volume fractions, respectively. s denotes the volume of one microscale element within a macroscale unit cell. With these two volume constraints applied on two scales, different types of design variables can be decoupled, which simplifies the sensitivity calculation and the updating of design variables.

A typical issue in topology optimization with minimization of dynamic compliance is that the material usually exhibit discontinuous distribution when an excitation frequency higher than the fundamental eigenfrequency is applied, with a very high level static compliance value (Olhoff and Du, 2014). Intuitively, a static constraint or other similar constraints reflecting the static stiffness

of structures can be introduced to deal with this issue and ensure the connectivity of optimized material layout (Olhoff and Du, 2016; Olhoff and Niu, 2016; Niu and Wadbro, 2021). In this research, the static constraint is chosen and can be formulated as

$$G^s = \int_{D^{\text{MA}}} \mathbf{g} \mathbf{u}_0 \delta(\phi) |\nabla \phi| d\Omega - J_S^* \leq 0, \quad (3.22)$$

where $\mathbf{u}_0$ is the displacement obtained via the static structural analysis, J_S^* is the maximum allowed static compliance value towards optimization results and $J_S^* = \vartheta \cdot J_S^0$, which is the product of a given parameter ϑ and the static compliance of a reference structure. In this paper, initial structures of numerical examples are selected as reference structures to get the J_S^0 . It should be noted that in the promising research of Silva et al. (Silva, Neves, and Lenzi, 2019), the static constraint is found not to be sufficient in ensuring final "0-1" material distribution when introduced into density-based dynamic compliance minimization, unless with a pretty severe value. Different from the density-based methods, the VFLS method in the proposed multiscale topology optimization framework can always achieve clear "0-1" macroscale material layout due to the level set function. As a result, discontinuous macroscale material distribution, rather than the intermediate density field, will appear in our research when considering excitation frequencies higher than the fundamental eigenfrequency. Therefore, the static constraint introduced in our topology optimization framework can ensure the continuity of material layout because a discontinuous macroscale material distribution will directly lead to a serious violation of the given static constraint.

Therefore, the mathematical model for the multiscale topology optimization can be constructed as

$$\begin{aligned} & \text{Min: } J_d, \\ & \text{s.t. } \begin{cases} a(\mathbf{u}, \mathbf{v}, \boldsymbol{\phi}) = l(\mathbf{v}, \boldsymbol{\phi}) \quad \forall \mathbf{v} \in U, \\ G^{\text{MA}} \leq 0, \\ G^{\text{MI}} \leq 0, \\ G^s \leq 0, \\ \underline{V}^n \leq V_j^n \leq \bar{V}^n, \\ 0 \leq \eta_i \leq 1, \end{cases} \end{aligned} \quad (3.23)$$

The flowchart of the proposed framework is shown in Fig. 3.3. In each iteration step, the microscale finite element analysis is firstly conducted for the evaluation of the homogenized elasticity tensor of macroscale unit cells by the energy-based homogenization method presented in Eq. (3.17). After obtaining the effective material densities of microstructures, the macroscale finite element analysis is performed to get the macroscale structural complex displacements. Next, the objective function value is computed based on Eq. (3.6), as well as the added volume constraints.

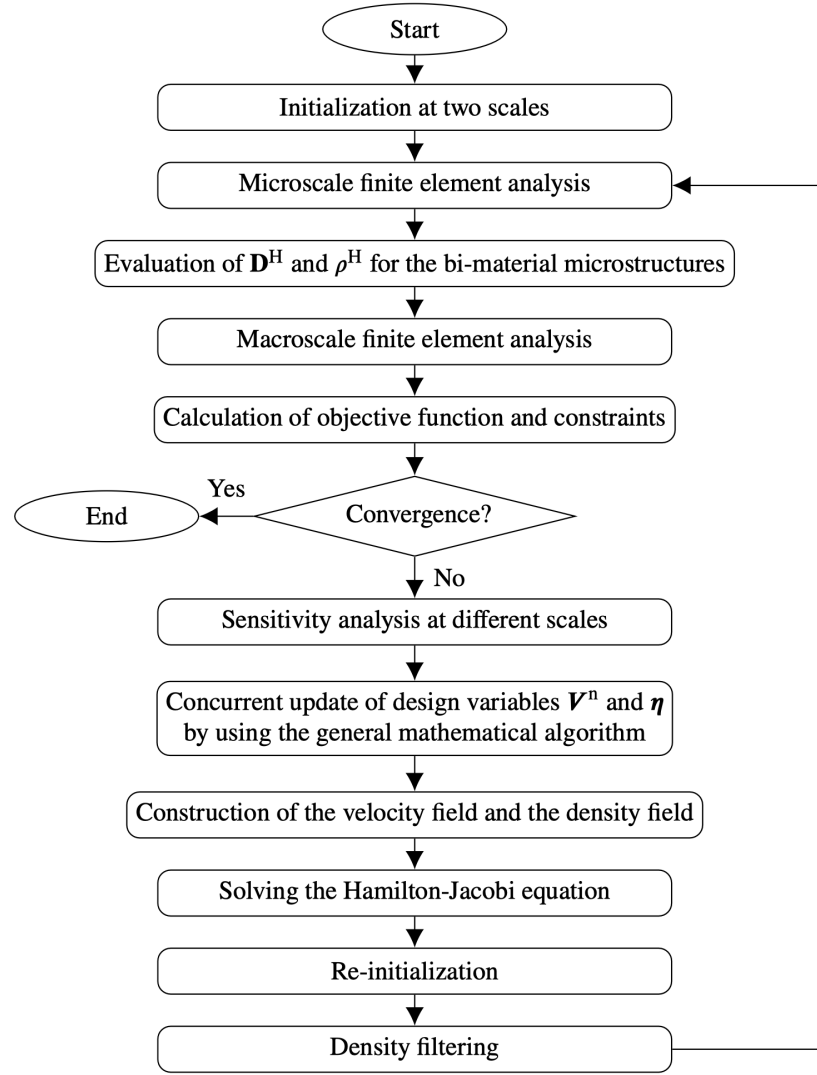


FIGURE 3.3: Optimization flowchart.

Then, the derivatives of the objective function and constraints with respect to macroscale and microscale design variables are calculated. Finally, the mathematical algorithm is employed and different types of the concerned design variables are concurrently updated, and thus the macrostructural and microstructural evolution can be achieved. The optimization process is repeated until the given convergence condition is satisfied.

It is worth noting that different types of design variables may lead to sensitivity at different orders of magnitude and cause some numerical difficulties. However, the optimization at two scales is respectively solved in our research, in which two Method of Moving Asymptotes (MMA) (Svanberg, 1987) algorithms are introduced to update different design variables separately. Therefore, the possible different orders of magnitude on sensitivity can be avoided.

Remark. Combining the advantages of different topology optimization methods has been presented for several times (Li, Luo, Gao, and Walker, 2018; Wang, Chen, and Wang, 2017; Wang and Kang, 2019; Liu, Kang, and Luo, 2020). In the proposed multiscale topology optimization method, the VFLS method is selected to deal with the distribution of multiple materials at the macroscale level, in which a more rigorous interpretation of the unit cell layout can be achieved and the uniform thickness of the outer coating can be easily maintained due to the signed distance property of the VFLS method. In addition, smooth structural boundaries can be obtained. At the microscale, we use the SIMP method to design layer-wise bi-material microstructures considering its simplicity of numerical implementation. Even though the microstructures we designed have unclear boundaries (which can be eliminated with special techniques, such as body-fitted mesh (Li, Kondoh, Jolivet, Furuta, Yamada, Zhu, Izui, and Nishiwaki, 2022)), the authors believe that achieving smooth structural boundaries in the bi-material lattice infilling of coated structures is of little importance and thus the designs we obtained are acceptable. Although the VFLS method and the SIMP method are combined in the proposed approach to conduct topology optimization at different scales, there are no fundamental difficulties in using only the VFLS method or the SIMP method for multiscale structural design. However, several filtering and projection operations (Clausen, Aage, and Sigmund, 2015; Clausen, Andreassen, and Sigmund, 2017; Luo, Li, and Liu, 2019) should be introduced into the density method-based macroscale topology optimization to identify the infilling and the coating. Besides, the unclear boundaries of the optimized macrostructures need to be post-processed, which may further causes the reduction of structural performance (Zuo, Xie, and Huang, 2010; Zhou and Rozvany, 1991). In addition, even though the SIMP-based multiscale topology optimization is easy to implement, the commonly used static constraint cannot ensure final "0-1" continuous material distribution when the excitation frequency is higher than the fundamental one, unless with a severe value (Silva, Neves, and Lenzi, 2019). For microscale topology optimization via the VFLS method, the computational cost is comparatively larger than the SIMP method. Furthermore, having no ability to nucleate holes, optimization results obtained via the VFLS method may exhibit worse structural performance than those of the SIMP method. Therefore, the concurrent multiscale topology optimization framework we proposed mixes the advantages of the VFLS method and the SIMP method to a large extent.

3.4 Sensitivity analysis

3.4.1 Macroscale sensitivity analysis

According to objective function for the minimization of the dynamic compliance Eq. (3.5), J_u can be rewritten as

$$J_u = \int_{D^{\text{MA}}} \left[(1 + i\omega\mathcal{B})\boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}^{\text{MA}} : \boldsymbol{\varepsilon}(\mathbf{u}) + (i\omega\mathcal{A} - \omega^2) \mathbf{u} \boldsymbol{\rho}^{\text{MA}} \mathbf{u} \right] H(\phi) d\Omega. \quad (3.24)$$

The material derivative of J_u can be expressed as

$$\begin{aligned} J'_u = & \int_{D^{MA}} \left[2(1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}') : \mathbf{D}^{MA} : \varepsilon(\mathbf{u}) + 2(i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{u} \right] H(\phi) d\Omega \\ & + \int_{\partial\Omega^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}) : \mathbf{D}^{MA} : \varepsilon(\mathbf{u}) V_n d\Gamma + \int_{\partial\Omega^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{u} V_n d\Gamma. \end{aligned} \quad (3.25)$$

Taking the material derivative on both sides of the state equation Eq. (3.1), we have the following equation:

$$\begin{aligned} & \int_{D^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}') : \mathbf{D}^{MA} : \varepsilon(\mathbf{v}) H(\phi) d\Omega + \int_{D^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}) : \mathbf{D}^{MA} : \varepsilon(\mathbf{v}') H(\phi) d\Omega \\ & + \int_{\partial\Omega^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}) : \mathbf{D}^{MA} : \varepsilon(\mathbf{v}) V_n d\Gamma + \int_{D^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}'\rho^{MA}\mathbf{v} H(\phi) d\Omega \\ & + \int_{D^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{v}' H(\phi) d\Omega + \int_{\partial\Omega^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{v} V_n d\Gamma \\ & = \int_{D^{MA}} \tilde{\mathbf{p}}\mathbf{v}' H(\phi) d\Omega + \int_{\partial\Omega^{MA}} \tilde{\mathbf{p}}\mathbf{v} V_n d\Gamma + \int_{\partial\Omega^{MA}} \mathbf{f}\mathbf{v}' d\Gamma + \int_{\partial\Omega^{MA}} [\nabla(\mathbf{f}\mathbf{v}) \cdot \mathbf{n} + \kappa(\mathbf{f}\mathbf{v})] V_n d\Gamma. \end{aligned} \quad (3.26)$$

Considering that $\mathbf{v}' \in U$, the following vibrational state equation can be obtained:

$$\begin{aligned} & \int_{D^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}) : \mathbf{D}^{MA} : \varepsilon(\mathbf{v}') H(\phi) d\Omega + \int_{D^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{v}' H(\phi) d\Omega \\ & = \int_{D^{MA}} \tilde{\mathbf{p}}\mathbf{v}' H(\phi) d\Omega + \int_{\partial\Omega^{MA}} \mathbf{f}\mathbf{v}' d\Gamma. \end{aligned} \quad (3.27)$$

Using the above equations, we have

$$\begin{aligned} & \int_{D^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}') : \mathbf{D}^{MA} : \varepsilon(\mathbf{v}) H(\phi) d\Omega + \int_{D^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}'\rho^{MA}\mathbf{v} H(\phi) d\Omega \\ & = \int_{\partial\Omega^{MA}} \tilde{\mathbf{p}}\mathbf{v} V_n d\Gamma + \int_{\partial\Omega^{MA}} [\nabla(\mathbf{f}\mathbf{v}) \cdot \mathbf{n} + \kappa(\mathbf{f}\mathbf{v})] V_n d\Gamma - \int_{\partial\Omega^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}) : \mathbf{D}^{MA} : \varepsilon(\mathbf{v}) V_n d\Gamma \\ & - \int_{\partial\Omega^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{v} V_n d\Gamma. \end{aligned} \quad (3.28)$$

Since the dynamic compliance problem is self-adjoint (Li, Luo, Gao, and Wu, 2018) and no body force is considered in this research, as well as the fixed edge that the excitation force is applied on, we can obtain the following equation:

$$J'_u = - \int_{\partial\Omega^{MA}} (1 + i\omega\mathcal{B})\varepsilon(\mathbf{u}) : \mathbf{D}^{MA} : \varepsilon(\mathbf{u}) V_n d\Gamma - \int_{\partial\Omega^{MA}} (i\omega\mathcal{A} - \omega^2) \mathbf{u}\rho^{MA}\mathbf{u} V_n d\Gamma. \quad (3.29)$$

Using the piece-wise function as the basis function, the sensitivity of J_u with respect to macroscale design variables can be derived as

$$\begin{aligned} \frac{\partial J_u}{\partial V^n} = & - \int_{\partial\Omega_{cv}} [(1 + i\omega\mathcal{B})\boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}_c : \boldsymbol{\varepsilon}(\mathbf{u}) + (i\omega\mathcal{A} - \omega^2) \mathbf{u}\boldsymbol{\rho}_c \mathbf{u}] p_j \, d\Gamma \\ & - \int_{\partial\Omega_{sc}} [(1 + i\omega\mathcal{B})\boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}^{MA} : \boldsymbol{\varepsilon}(\mathbf{u}) + (i\omega\mathcal{A} - \omega^2) \mathbf{u}\boldsymbol{\rho}^{MA} \mathbf{u}] p_j \, d\Gamma. \end{aligned} \quad (3.30)$$

For coated structures, the material interface consists of two parts, i.e., the boundary between the coating and the void region $\partial\Omega_{cv}$, and the boundary between the coating and the substrate area $\partial\Omega_{sc}$ ($\partial\Omega^{MA} = \partial\Omega_{cv} \cup \partial\Omega_{sc}$), and the variation of them must be considered in the derivation of the shape derivative. We denote the last term on the right side of the above equation as T_1 , then we have

$$T_1 = \int_{\partial\Omega_{cv}} g_1 |\det(\mathbf{I} - b_c \nabla \mathbf{n})| p_j \, d\Gamma = \int_{\partial\Omega_{cv}} g_1 \prod_{i=1}^{N'-1} (1 - b_c \kappa_i) p_j \, d\Gamma, \quad (3.31)$$

where,

$$g_1 = \begin{cases} 0 & , \text{if } \mathbf{x} - b_c \mathbf{n} \notin \partial\Omega_{sc} \\ (1 + i\omega\mathcal{B}) \|\boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}^{MA} : \boldsymbol{\varepsilon}(\mathbf{u})\|_{\Delta} & \mathbf{x} \in \partial\Omega_{cv}, \\ + (i\omega\mathcal{A} - \omega^2) \mathbf{u} \|\boldsymbol{\rho}^{MA}\|_{\Delta} \mathbf{u}|_{\mathbf{x}-b_c \mathbf{n}}, & \text{if } \mathbf{x} - b_c \mathbf{n} \in \partial\Omega_{sc}, \end{cases} \quad (3.32)$$

where $\|Q(x)\|_{\Delta}$ is the normal-directional jump of the function $Q(x)$ across the boundary Ω_{sc} , i.e., $\|Q(x)\|_{\Delta} = Q(x)_{-0} - Q(x)_{+0}$ (Wang and Kang, 2018a).

The sensitivity formulation of J_u with respect to macroscale design variables can be formulated as

$$\frac{\partial J_u}{\partial V^n} = - \int_{\partial\Omega_{cv}} [(1 + i\omega\mathcal{B})\boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{D}_c : \boldsymbol{\varepsilon}(\mathbf{u}) + (i\omega\mathcal{A} - \omega^2) \mathbf{u}\boldsymbol{\rho}_c \mathbf{u}] p_j \, d\Gamma - \int_{\partial\Omega_{cv}} g_1 \prod_{i=1}^{N'-1} (1 - b_c \kappa_i) p_j \, d\Gamma, \quad (3.33)$$

where N' is the dimensionality, and $\kappa_i (1 \leq i \leq N' - 1)$ are the principal curvatures.

Finally, the sensitivity of the objective function J_d with respect to macroscale design variables can be yielded as

$$\begin{aligned} \frac{\partial J_d(\Omega_\theta)}{\partial V^n} &= \frac{\partial J'_d(\Omega)(\theta)}{\partial V^n} \\ &= \frac{1}{J_d} \left[\text{real}(J_u) \text{real}\left(\frac{\partial J_u}{\partial V^n}\right) + \text{imag}(J_u) \text{imag}\left(\frac{\partial J_u}{\partial V^n}\right) \right]. \end{aligned} \quad (3.34)$$

The sensitivity of the static compliance constraint is skipped here for saving space, which can be regarded as a special case of the above derivation by replacing $\mathbf{f}$ and $\mathbf{u}$ with $\mathbf{f}_0$ and $\mathbf{u}_0$ with the

setting $\omega = 0$ (Niu and Wadbro, 2021).

Sensitivities of volume constraints at two scales with respect to macroscale design variables can be respectively expressed as

$$\frac{\partial G^{\text{MA}}}{\partial V^n} = \int_{D^{\text{MA}}} \delta(\phi) |\nabla \phi| p_j \, d\Omega, \quad (3.35a)$$

$$\frac{\partial G^{\text{MI}}}{\partial V^n} = \sum_{l=1}^L \int_{D_l^{\text{MA}}} \left(\sum_{e=1}^{n^{\text{MI}}} x_l^e s_l^e / |\mathbf{Y}| \right) \delta(\phi - b_c) |\nabla \phi| p_j \, d\Omega - f^{\text{MI}} \int_D \delta(\phi - b_c) |\nabla \phi| p_j \, d\Omega. \quad (3.35b)$$

3.4.2 Microscale sensitivity analysis

Similarly, the sensitivity analysis of the design objective with respect to microscale design variables η can be formulated as

$$\frac{\partial J_d}{\partial \eta} = \frac{1}{J_d} \left[\text{real}(J_u) \, \text{real} \left(\frac{\partial J_u}{\partial \eta} \right) + \text{imag}(J_u) \, \text{imag} \left(\frac{\partial J_u}{\partial \eta} \right) \right], \quad (3.36)$$

where,

$$\frac{\partial J_u}{\partial \eta} = \int_{D^{\text{MA}}} \left[2(1 + i\omega \mathcal{B}) \boldsymbol{\varepsilon}(\mathbf{u}) \cdot \frac{\partial \mathbf{D}^{\text{H}}}{\partial \eta} \cdot \boldsymbol{\varepsilon}(\mathbf{u}) + 2(i\omega \mathcal{A} - \omega^2) \mathbf{u} \frac{\partial \boldsymbol{\rho}^{\text{H}}}{\partial \eta} \mathbf{u} \right] d\Omega. \quad (3.37)$$

The sensitivity of $\mathbf{D}^{\text{H}}$ with respect to microscale design variables η is formulated as

$$\frac{\partial \mathbf{D}^{\text{H}}}{\partial \eta} = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} \frac{\partial \mathbf{D}^{\text{MI}}}{\partial \eta} \boldsymbol{\varepsilon}_{pq}^{A(\tilde{i}\tilde{j})} \boldsymbol{\varepsilon}_{rs}^{A(\tilde{k}\tilde{l})} d\mathbf{y} \quad \tilde{i}, \tilde{j}, p, q = 1, 2, \dots, d, \quad (3.38)$$

where,

$$\frac{\partial \mathbf{D}^{\text{MI}}}{\partial \eta} = \varsigma \eta^{\varsigma-1} (\mathbf{D}_1 - \mathbf{D}_2). \quad (3.39)$$

The sensitivity of $\boldsymbol{\rho}^{\text{H}}$ with respect to microscale design variables η is calculated as

$$\frac{\partial \boldsymbol{\rho}^{\text{H}}}{\partial \eta} = \frac{1}{|\mathbf{Y}|} (\mathbf{D}_1 - \mathbf{D}_2). \quad (3.40)$$

Similar to the macroscale case, the sensitivity for limiting the static compliance of structures can be calculated based on above equations.

The sensitivity of volume constraints at two scales with respect to microscale design variables η can be expressed as

$$\frac{\partial G^{\text{MA}}}{\partial \eta} = 0, \quad (3.41a)$$

$$\frac{\partial G^{\text{MI}}}{\partial \eta_l^e} = \int_{D_l^{\text{MA}}} [s_l^e / |\mathbf{Y}_l|] H(\phi - b_c) d\Omega. \quad (3.41b)$$

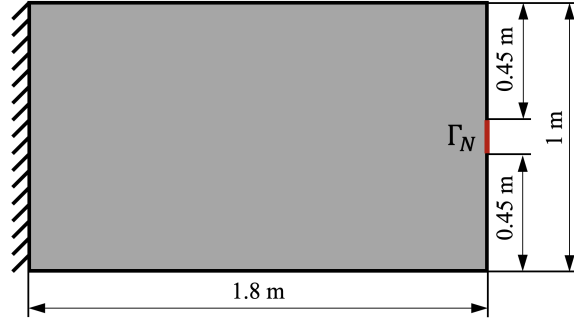


FIGURE 3.4: The structure setup for the cantilever beam

3.5 Numerical examples

This section provides various numerical examples in two dimensions to verify the effectiveness of the proposed method, which covers different structural setups, different thicknesses of the outer coating, different numbers of divided layers for the lattice infill, different element sizes at two scales, etc. In all numerical examples, layers for the lattice infill area are uniformly (or near-uniformly) divided along a specific direction. Without extra specification, each unit cell in the macrostructure is discretized into 40×40 uniformly-sized planar square bi-linear microscale elements. To conduct macroscale finite element analysis, 5×5 Gauss integration points are distributed within each macroscale element and then the coating thickness smaller than one macroscale element can be well considered. The density filtering technique (Bourdin, 2001) is adopted to avoid checkerboard or mesh-dependency problems with a filter radius $r_{min} = 2$. All microstructures presented in the sequence from left to right are for the macroscale layer of the substrate from bottom to top, unless otherwise stated. Besides, all optimized microstructures are presented in a 3-by-3 repetition for better illustration. The MMA algorithm is used to solve the optimization problems at two scales and only in-plane vibration is considered. The iteration will terminate when: (1) five previous values of the objective function during the iteration differ by less than $1e-3$, and (2) the relative difference between the adjacent two objective function values is not greater than $1e-4$.

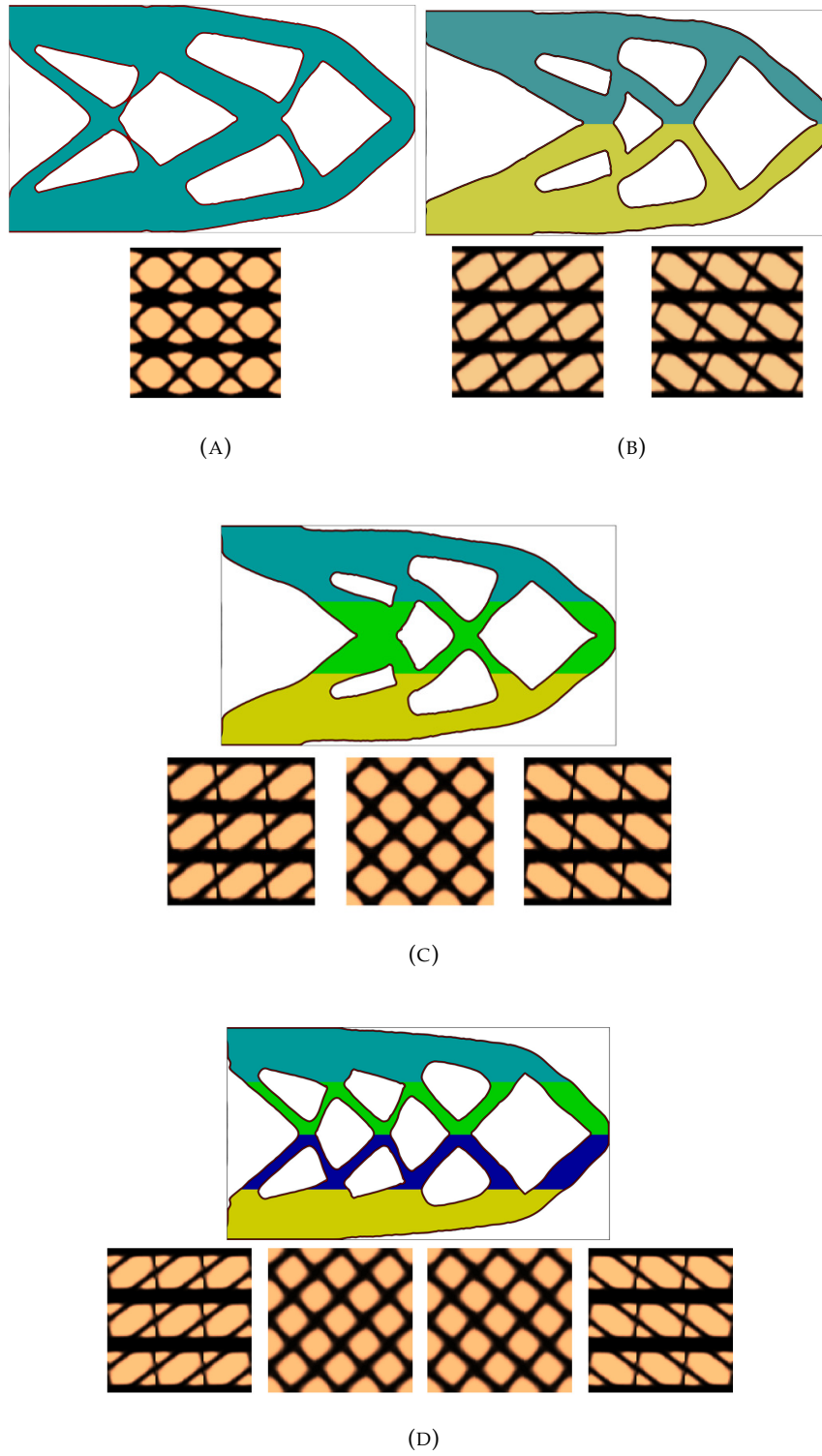


FIGURE 3.5: Macroscale and microscale optimization results for the cantilever beam infilled with (a) one-layer lattice infill; (b) two-layer lattice infill; (c) three-layer lattice infill; (d) four-layer lattice infill.

3.5.1 Cantilever beam

A cantilever beam structure is studied as the first example, whose length and height are 1.8 m and 1 m, respectively. The macrostructure is discretized into 180×100 finite number of elements. The thickness of the coating is set as $6.0 \cdot 10^{-3}$ m. In terms of material properties, Young's modulus for the coating, the microscale base material 1, and the microscale base material 2 for the bi-material lattice infill are respectively defined as $E_c = 5$ GPa, $E_1 = 3$ GPa, and $E_2 = 0.01$ GPa. As for the material densities, we set $\rho_c = 7800$ kg/m³, $\rho_1 = 5600$ kg/m³, and $\rho_2 = 1500$ kg/m³ respectively for the coating, the base material 1, and the base material 2. A distributed time-harmonic excitation force is applied on the boundary Γ_N (N refer to "Neumann"), marked in red as shown in Fig. 3.4, with an excitation frequency of 5 Hz. The maximum volume fractions f^{MA} and f^{MI} are all set as 50%.

Considering different layers for the lattice infill

To test the potential of layer-wise bi-material lattice infill for coated structures, we consider several cases of lattice microstructures, including one-layer (uniform and periodic), two-layer, three-layer, and four-layer lattice infilling, with the structural damping coefficients assumed as $\mathcal{A} = 5\text{e-}3$ and $\mathcal{B} = 1\text{e-}4$. The optimization results at two scales are presented in Fig. 3.5. It can be observed that considering different layers of lattice infill microstructures can lead to varied macrostructural topologies. All macrostructures we obtained have clear and smooth boundaries. Besides, the outer coating with uniform thickness is well-described in all cases thanks to the maintenance of the signed distance property. At the microscale, the boundaries of different materials in the bi-material lattice structures are clear. With consideration of different numbers of divided layers, various microstructural patterns are concurrently optimized with the evolution of their macrostructures. Moreover, microstructural configurations at the top and the bottom layer are symmetric with each other according to the symmetry of macroscale coated structures.

Although the macrostructures infilled with two layers (Fig. 3.5b) and three layers (Fig. 3.5c) of bi-material lattice infilling share some similarities, a new type of microstructural pattern is obtained for the second layer in the three-layer case, which contributes a lower dynamic compliance value ($5.16 \cdot 10^{-2} \text{N} \cdot \text{m}$) than that of the optimized macrostructure infilled with a two-layer lattice structure ($5.40 \cdot 10^{-2} \text{N} \cdot \text{m}$). The optimized macrostructure infilled with periodic and uniform bi-material lattice infill has a final dynamic compliance $5.52 \cdot 10^{-2} \text{N} \cdot \text{m}$ and the four-layer consideration for the bi-material lattice leads to a final value of the objective function as $4.81 \cdot 10^{-2} \text{N} \cdot \text{m}$. An interesting phenomenon appears in this example that no new microstructural patterns are optimized by adding one more layer for the bi-material lattice infill based on the three-layer case. However, the macroscale topologies between the three-layer case and the four-layer case are different. To be specific, more truss-like structures are obtained in the former one than that of the

TABLE 3.1: Comparison of dynamic compliance of optimized coated cantilever beams.

Layers of the lattice infill	1	2	3	4
Dynamic compliance value ($\text{N} \cdot \text{m}$)	$5.52 \cdot 10^{-2}$	$5.40 \cdot 10^{-2}$	$5.16 \cdot 10^{-2}$	$4.81 \cdot 10^{-2}$

latter one, which reveals the importance of performing a concurrent multiscale topology optimization strategy.

Through this coated cantilever beam, it is found that different numbers of divided layers for the bi-material lattice microstructures have the ability to generate different macroscale and microscale topologies. Also, the macroscale and microscale configurations have a strong interference between each other during the iteration. In addition, the more divided the layers for the lattice infill, the lower final dynamic compliance can be obtained by using the proposed method.

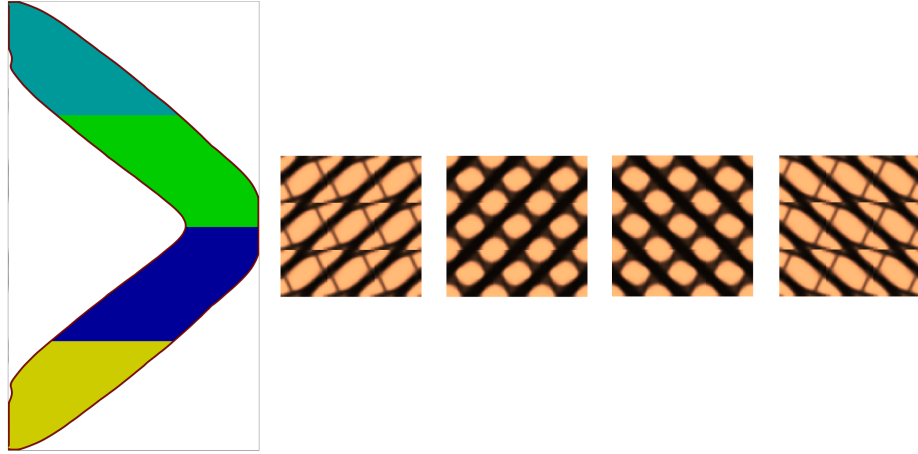


FIGURE 3.6: Macroscale and microscale optimization results for the cantilever beam of different structural dimensions, infilled with a four-layer lattice infill.

Considering different structural dimensions

In this subsection, the dimensions of the cantilever beam structure shown in Fig. 3.4 is interchanged, i.e., rotating the structure of 90 degrees. The volume fractions at two scales f^{MA} and f^{MI} are set as 40% and 50%, respectively. The material properties and other design parameters are remained the same, with the microstructural infilling divided into four layers. The macroscale and microscale optimization results are shown in Fig. 3.6 with a dynamic compliance value as $8.21 \cdot 10^{-3} \text{N} \cdot \text{m}$. It can be observed that the optimized macrostructure still has smooth structural boundaries with the well-maintained coating thickness. However, compared to the non-rotated result shown in Fig. 3.5d, the macrostructural configuration exhibits great difference as no truss-like structural characteristics are obtained. At the microscale level, the microstructures for the middle two layers are similar to those presented in Fig. 3.6. As for the top and the bottom layers,

optimized microstructures present new topologies with several inclined bars and no horizontal distribution of the base material 1 appears. Through this numerical example, it is proved that the dimension of macroscale structures can affect the optimization results at two scales.

Considering different damping coefficients

To investigate the influence of damping coefficients on optimization results, we consider two groups of coefficients in this subsection, i.e., $\mathcal{A} = 1$, $\mathcal{B} = 1\text{e-}2$, and $\mathcal{A} = 1\text{e-}1$, $\mathcal{B} = 5\text{e-}3$. It should be noted that the optimization results are not sensitive to the variation of damping coefficients when the applied excitation frequency is lower than the fundamental eigenfrequency (Silva, Neves, and Lenzi, 2019; Niu and Wadbro, 2021) and thus only "high" excitation frequency is considered here. The static constraint is set as $J_S^* = 10J_S^0$. The maximum volume fractions f^{MA} and f^{MI} are set as 40% and 50%, respectively. The thickness of the coating and material properties are the same as in Section 3.5.1. The excitation of 120 Hz is considered and the lattice infilling is divided into two layers. The optimization results at different scales with varied damping coeffi-

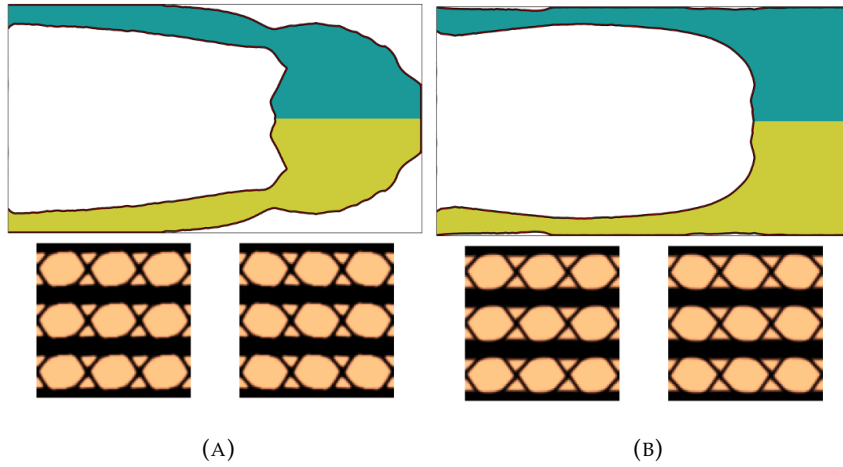


FIGURE 3.7: Macroscale and microscale optimization results for the cantilever beam infilled with a two-layer lattice infill with different damping coefficients: (a) $\mathcal{A} = 1$ and $\mathcal{B} = 1\text{e-}2$; (b) $\mathcal{A} = 1\text{e-}1$ and $\mathcal{B} = 5\text{e-}3$.

icients are presented in Fig. 3.7. At the macroscale level, it can be observed that macrostructures we obtained show some similarities. However, compared to the higher damping coefficients case, there is much more material accumulated around the right boundary, as shown in Fig. 3.7b. As for the microscale, similar microstructural patterns are obtained with clear bi-material distribution. It should be noted that the dynamic compliance value is expected to be lower when a set of higher damping coefficients is applied, under the same dynamic excitation force. However, the dynamic compliance of the optimized design presented in Fig. 3.7a is $1.10 \cdot 10^{-2} \text{N} \cdot \text{m}$, which is higher than that of the lower damping coefficients case ($1.06 \cdot 10^{-2} \text{N} \cdot \text{m}$). This indicates the optimization result shown in Fig. 3.7a is a local optimum but the proposed scheme can still generate effective

optimization results for the minimization of dynamic compliance. With this comparison, it can be concluded that different damping coefficients can lead to different macroscale topologies but may have limited influence on the optimized microstructures using the proposed multiscale topology optimization framework.

Considering different static constraints

Based on the previous example, the coated cantilever beam with damping coefficients $\mathcal{A} = 1$ and $\mathcal{B} = 1\text{e-}2$ is selected here to test the effect of static constraints on the final optimization results. The excitation frequency is defined as 150 Hz. The optimized designs with static constraints $J_S^* = 10J_S^0$ and $J_S^* = 15J_S^0$ are obtained and shown in Fig. 3.8a and Fig. 3.8b, respectively. In general, the macrostructures considering different static constraints we obtained have similar material layout. However, there are some small holes exhibited in the optimized macrostructure presented in Fig. 3.8a. Besides, it has less macroscale material distribution in the right part of the domain. These varied macrostructural characteristics contribute certain stiffness under the limitation of the static compliance. In Fig. 3.8b, the structure at the macroscale level is similar to the macrostructure shown in Fig. 3.7b. From figures shown in Fig. 3.8, the final designs at the microscale share great similarities. The objective values of structures considering $J_S^* = 10J_S^0$ and $J_S^* = 15J_S^0$ are $7.65 \cdot 10^{-3} \text{N} \cdot \text{m}$ and $7.13 \cdot 10^{-3} \text{N} \cdot \text{m}$, respectively. Therefore, it can be concluded that the dynamic compliance of the coated structure with lattice infill is decreased with a larger bound on the static compliance using the proposed approach.

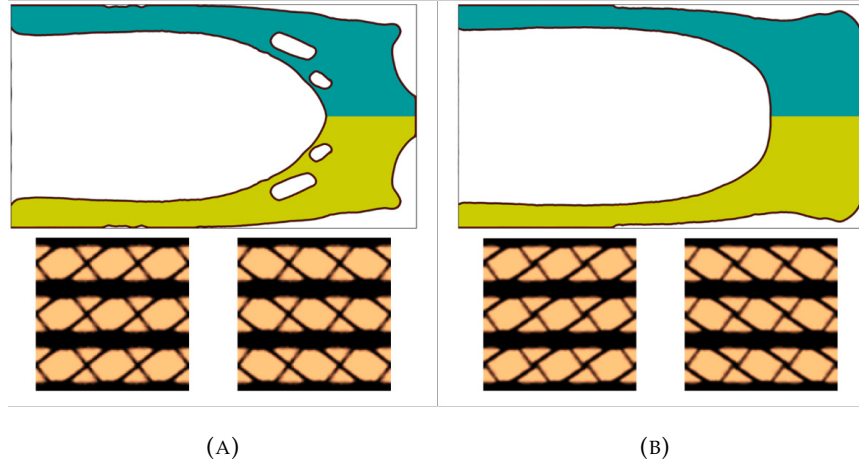


FIGURE 3.8: Macroscale and microscale optimization results for the cantilever beam infilled with a two-layer lattice infill with different static constraints: (a) $J_S^* = 10J_S^0$; (b) $J_S^* = 15J_S^0$.

3.5.2 MBB beam

In this example, we consider a MBB (Messerschmitt-Bölkow-Blohm) beam structure which is modified from the classical MBB beam. The length of the structure is 3 m and the height is 1 m, as presented in Fig. 3.9. The macrostructure is discretized into 300×100 finite number of elements. For the coating, Young's modulus is $E_c = 4$ GPa and the density is $\rho_c = 2000$ kg/m³. For the bi-material lattice, parameters set for Young's modulus are $E_1 = 3.5$ GPa and $E_2 = 0.05$ GPa, and those for material densities are $\rho_1 = 1800$ kg/m³ and $\rho_2 = 250$ kg/m³. The mass-proportional and stiffness-proportional damping coefficients $\mathcal{A}$ and $\mathcal{B}$ are defined as $5e-3$ and $1e-4$, respectively. As shown in Fig. 3.9, the excitation force is applied on the boundary Γ_N , which occupies $1/60$ of the top side of the design domain.

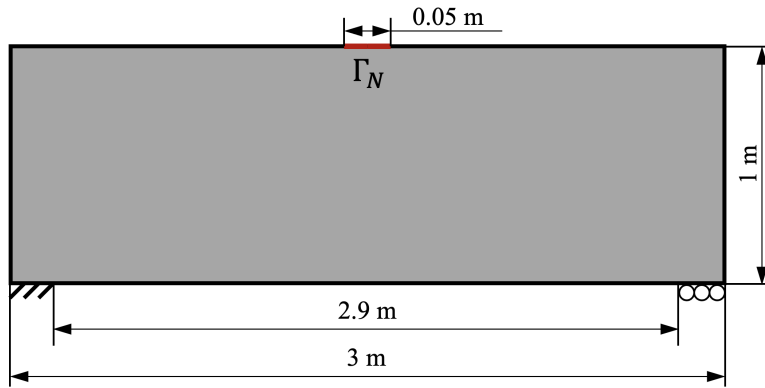


FIGURE 3.9: The structure setup for the MBB beam (whose ratio of length to height is 3)

Considering different coating thicknesses

Firstly, we study the influence of coating thickness on macroscale and microscale optimization results. The infilling of the coated MBB beam is divided into two layers. The maximum allowed volume fractions at two scales are set as $f^{MA}=45\%$ and $f^{MI}=50\%$, respectively. Under the same excitation frequency, two thicknesses of the outer coating are specified for the MBB beam structure, i.e., $1.0 \cdot 10^{-2}$ m and $1.5 \cdot 10^{-2}$ m.

In Fig. 3.10a and Fig. 3.11a, the obtained macrostructures are similar for different thicknesses of the outer coating. However, it can be seen that the macrostructure with the coating of $1.0 \cdot 10^{-2}$ m has some holes generated due to the merging of the coating. In Fig. 3.11a, the truss-like structures in the upper part of the structure are pretty slim and no holes emerged. At the microscale level, the microstructures we obtained are varied from each other in two different cases. For the case of $1.0 \cdot 10^{-2}$ m, the microstructure for the bottom layer comprises much more base material 1, which forms some thicker horizontal bars and some circle rings. Differently, the material distribution of the base material 1 in the microstructural topology for the top layer of the macrostructure shows

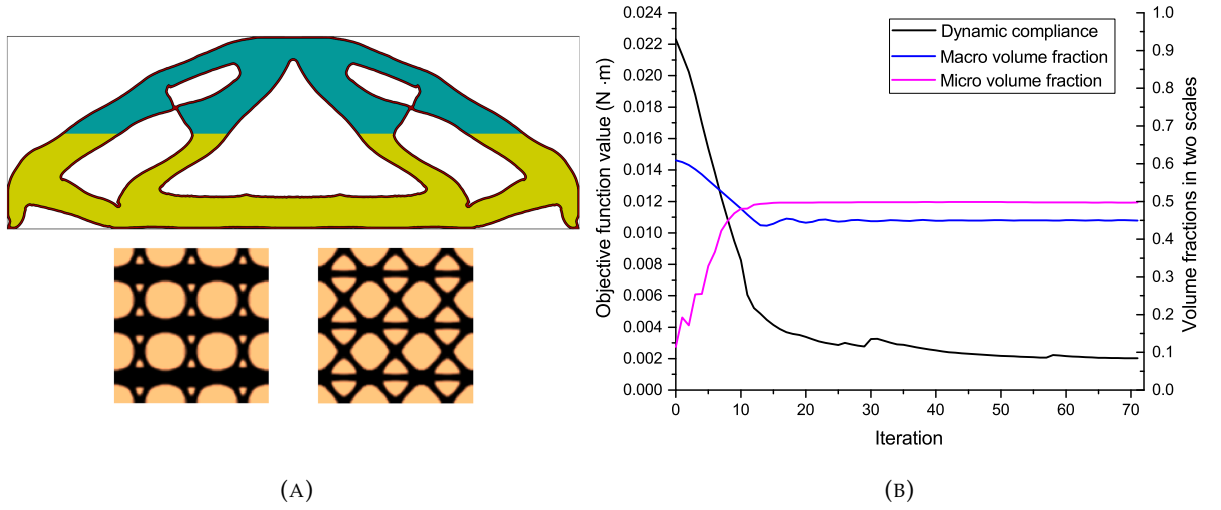


FIGURE 3.10: The MBB beam with a coating of $1.0 \cdot 10^{-2} \text{m}$, infilled with a two-layer lattice infill: (a) macroscale and microscale optimization results; (b) iteration history.

many horizontal and inclined straight bars. As for the macrostructure with the coating of a thicker thickness shown in Fig. 3.11a, the topologies of microstructures are almost the same but the one for the top layer consumes more base material 1, which is opposite from the case of $1.0 \cdot 10^{-2} \text{m}$. Generally, this phenomenon can be attributed to the interaction of structural evolution at two scales during the iteration.

The iteration histories for the coated MBB beam considering different thicknesses of the coating are presented in Fig. 3.10b and Fig. 3.11b, respectively. In both two cases, the value of the dynamic compliance decreases significantly during the first 20 iteration steps and gradually stabilize in the following iteration. Finally, the optimization for the $1.0 \cdot 10^{-2} \text{m}$ and $1.5 \cdot 10^{-2} \text{m}$ case terminates when the dynamic compliance reaches $2.02 \cdot 10^{-3} \text{N} \cdot \text{m}$ and $1.64 \cdot 10^{-3} \text{N} \cdot \text{m}$, respectively. The considered two volume constraints are both well satisfied and reach their maximum allowed values.

Considering different excitation frequencies

In this subsection, two different excitation frequencies, 5 Hz and 45 Hz (respectively smaller and larger than the fundamental eigenfrequency), are applied on the MBB beam to test how the value of excitation frequency can affect the optimization results at two scales. The thickness of the coating is set as $1.0 \cdot 10^{-2} \text{m}$ and periodic and uniform lattice infill is assumed. The upper volume limits for the macrostructural configuration f^{MA} and for the base material 1 in the microstructure f^{MI} are both set as 50 %. The static constraint is considered as $J_S^* = 5J_S^0$.

The optimization results at two scales are shown in Fig. 3.12a and Fig. 3.12b, respectively. It

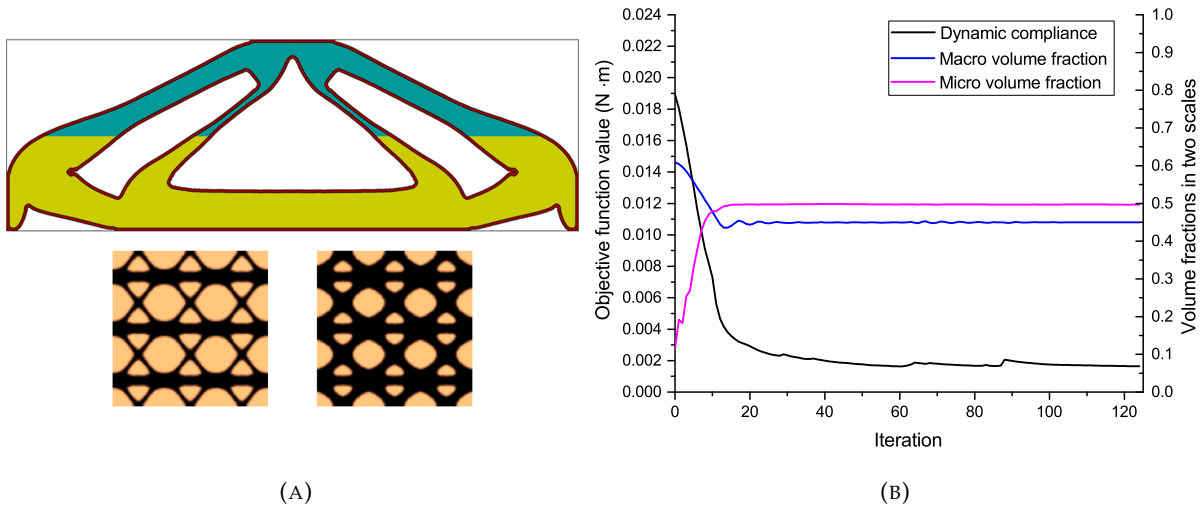


FIGURE 3.11: The MBB beam with a coating of $1.5 \cdot 10^{-2}\text{m}$, infilled with a two-layer lattice infill: (a) macroscale and microscale optimization results; (b) iteration history.

can be clearly seen that different excitation frequencies of the dynamic force lead to varied optimized macrostructures. For the case of excitation frequency 5 Hz, the macrostructure we obtained has many truss-like structures and some material is distributed at the bottom of the design domain. However, the macrostructural configuration obtained under the frequency of 45 Hz shows a arch bridge-like topology. It has fewer truss-like structures and no material distribution appears at the bottom of the domain, except around the fixed boundaries. The most obvious difference between these two structures can be observed that the macrostructure presented in Fig. 3.12a has a void area in the center of the design domain but most material accumulated in the central area of the one presented in Fig. 3.12b, which reveals that different excitation frequencies have a strong influence on the optimized designs. As for the outer coating, we can observed that the thicknesses of the coating are well-maintained in two cases and smooth boundaries are generated. There is no huge difference on the topologies of microstructures considering different excitation frequencies in this example. The dynamic compliance value of the structure shown in Fig. 3.12a is $2.08 \cdot 10^{-3}\text{N} \cdot \text{m}$ and the one shown in Fig. 3.12b is $2.32 \cdot 10^{-4}\text{N} \cdot \text{m}$.

Considering different initial microstructural guesses

Then, we study how the initial microstructural guess can affect the optimization results at two scales. Based on the setting of the numerical example presented in Fig. 3.12a, a different initial microstructural guess is given whose densities continuously change from "0" on the boundaries to "1" at the central point, as shown in Fig. 3.13a. The optimization result at two scales are presented in Fig. 3.13b, with the objective function value as $1.94 \cdot 10^{-3}\text{N} \cdot \text{m}$. It can be observed that macrostructures given in Fig. 3.12a and Fig. 3.13b are almost the same. However, there are

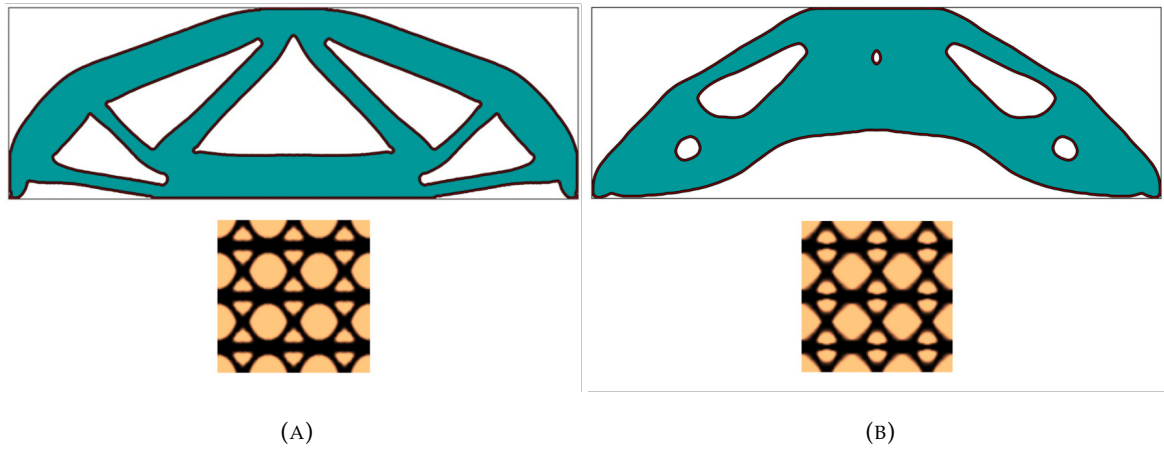


FIGURE 3.12: Macroscale and microscale optimization result for the MBB beam with different excitation frequencies: (a) 5 Hz; (b) 45 Hz.

some coating materials distributed within the substrate area of the macrostructural configuration in Fig. 3.13b, which might be generated due to different homogenized elasticity tensors during the iteration. Obviously, the microstructure we designed shown in Fig. 3.13b with a different initial microstructural guess varies from the previous one, in which some vertical bars made of the base material 1 are obtained, proving the dependency of optimized microstructures on their initial guesses.

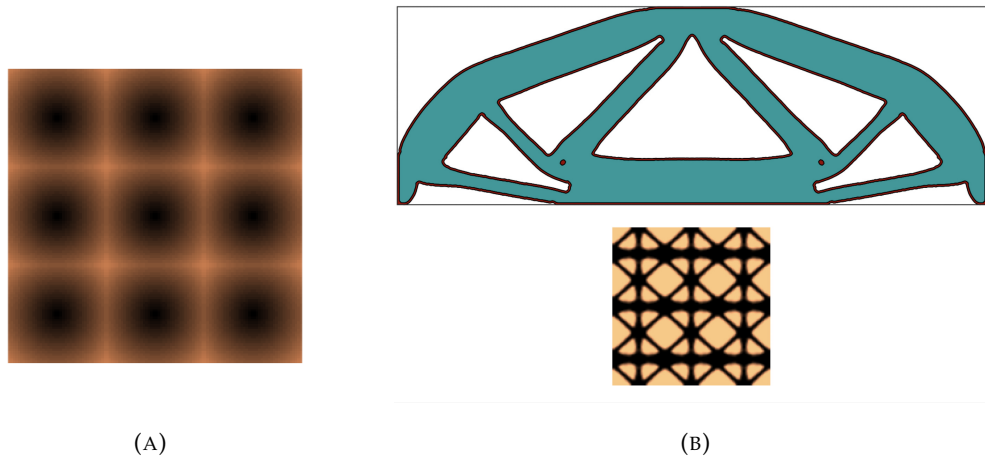


FIGURE 3.13: The MBB beam with a different initial microstructural guess: (a) the initial density distribution of the unit cell; (b) macroscale and microscale optimization result.

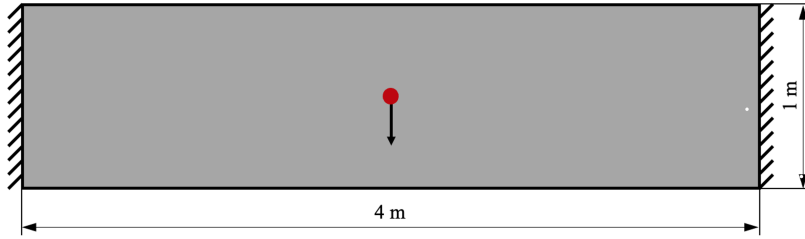


FIGURE 3.14: The structure setup for the clamped ends beam

3.5.3 Clamped ends beam

Considering different meshes

Finally, a clamped ends beam shown in Fig. 3.14 is considered to investigate the influence of different meshes, whose height and length are 1 m and 4 m, respectively. The thickness of the coating is set as $1.2 \cdot 10^{-2}$ m and four layers of lattice infill are studied. A downward harmonic excitation force is applied at the center of the macro design domain with the frequency of 10 Hz. Parameters for material properties are all given the same as those in the MBB example. The maximum volume fractions f^{MA} and f^{MI} for two scales are set as 45% and 50%, respectively. Two couples of element meshes are introduced: (1) 400×100 macroscale mesh and 40×40 microscale mesh, and (2) 800×200 macroscale mesh and 50×50 microscale mesh.

The macroscale and microscale optimization results with different meshes at two scales are shown in Fig. 3.15. Generally, the macroscale topologies and microstructural configurations in both cases are highly similar. Both macrostructures we optimized have smooth structural boundaries and several macro trusses are generated. However, much smoother material distribution is obtained in the macroscale structural configuration presented in Fig. 3.15b. At the microscale level, lattice structures for different layers exhibit clear material distribution and are symmetric due to the macroscale and microscale geometrical symmetry. Nevertheless, some varied features can be observed. For the first and fourth layers, there is less microscale base material 1 distribution in the horizontal black area in the finer mesh case (Fig. 3.15b) than that in the coarse mesh case (Fig. 3.15a). Although the main microscale topologies are the same, much more base material 1 appears on those slanted trusses in the second and third layers to reach the maximum microscale volume constraint. The final dynamic compliance values of the optimization results shown in Fig. 3.15a and Fig. 3.15b are $1.32 \cdot 10^{-3} \text{N} \cdot \text{m}$ and $1.44 \cdot 10^{-3} \text{N} \cdot \text{m}$, respectively. Despite some structural differences at two scales and an 8% gap between optimized dynamic compliance values, it is confirmed that the finer element meshes can lead to finer geometrical features, and the proposed concurrent multiscale topology optimization method has low mesh-dependency performance.

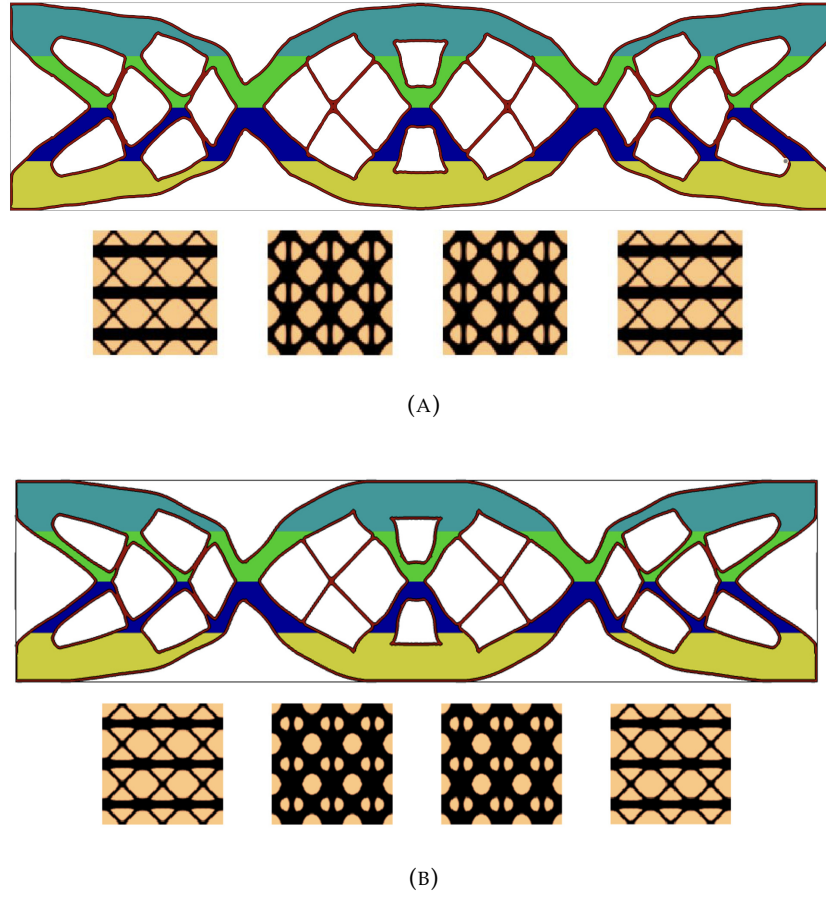


FIGURE 3.15: Macroscale and microscale optimization results for the clamped ends beam infilled with a four-layer lattice microstructure with (a) macroscale element mesh: 400×100 and microscale element mesh: 40×40 ; (b) macroscale element mesh: 800×200 and microscale element mesh: 50×50 .

Considering different direction for the layer-wise lattice infill

In the above numerical examples, the substrate area of coated structures are all horizontally divided into several layers for different topologies of bi-material lattice microstructures. In this example, we consider a different direction for the layer-wise lattice infill to test its influence towards the optimization results. In Fig. 3.16, the obtained macroscale structure considering vertically divided lattice infill still has smooth and clear boundaries and microstructures for different layers all exhibit well defined material distribution. However, various structural characteristics can be observed with the consideration of different directions for the lattice infill microstructures. At the macroscale level, much more material accumulate near the ends of the beam structure infilled with vertically-divided lattice to better resist the vibration and leads to stronger truss-like structures, compared to those shown in Fig. 3.15. Besides, the change of the division direction for the lattice microstructures causes variations towards microstructural configurations. The topologies of microstructures shown in Fig. 3.16 for the leftest layer and the rightest layer have much more base material 1 distribution. As for the middle two layers, truss-like structures composed of base material 1 are formed and much more base material 2 contributes the lattice microstructures, compared to the other layers. The final dynamic compliance value of the structure presented in Fig. 3.16 is $1.58 \cdot 10^{-3} \text{N} \cdot \text{m}$, which is larger than those of optimization results considering horizontally-divided lattice infill microstructures. This result reveals that the division direction for the layer-wise lattice infill has certain influence towards the performance of optimization results and should be carefully selected before performing concurrent multiscale topology optimization for coated structures.

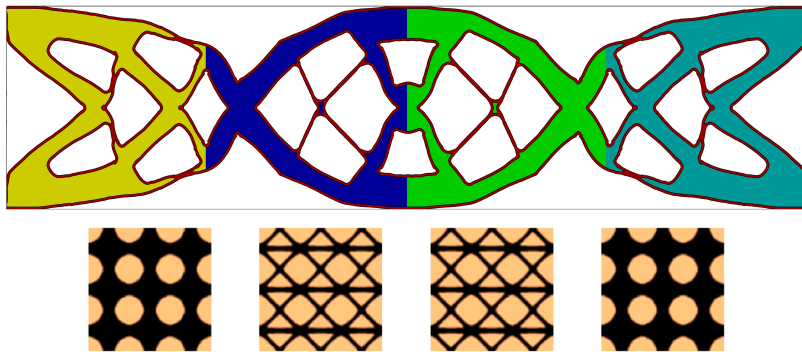


FIGURE 3.16: Macroscale and microscale optimization results for the clamped ends beam infilled with the vertically divided four-layer bi-material lattice microstructures.

Performance verification based on body-fitted mesh

To verify the performance of optimization results and check whether there exists local vibration areas in the lattice infill, a single-scale model of the optimized clamped ends beam is constructed based on the optimization results at two scales shown in Fig. 3.15a, in which those bi-material

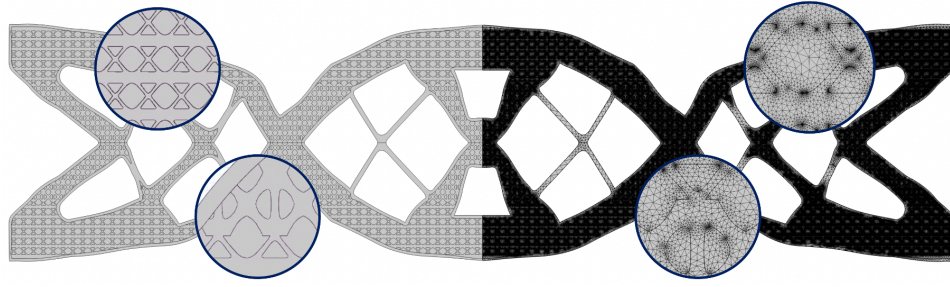


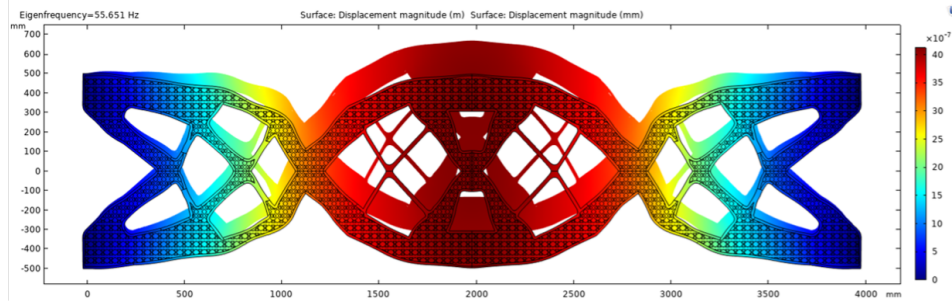
FIGURE 3.17: Geometrical model of the optimized clamped ends beam and its body-fitted mesh.

TABLE 3.2: Comparison of eigenfrequencies of the optimized coated clamped ends beam.

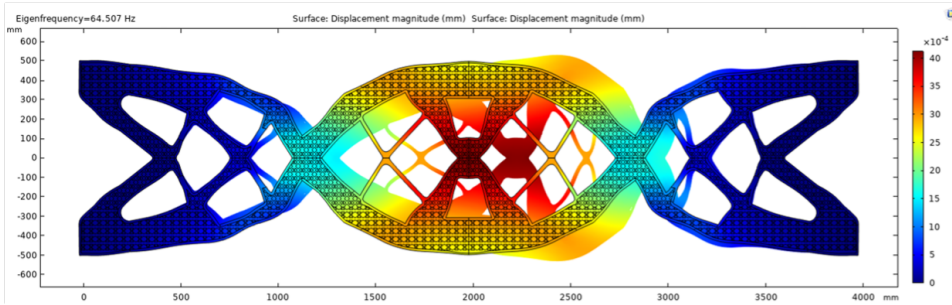
Order of eigenfrequencies	COMSOL	MATLAB	Difference
1st	55.651 Hz	50.034 Hz	10.093 %
2nd	64.507 Hz	57.519 Hz	10.833 %
3rd	82.463 Hz	73.100 Hz	11.354 %

lattice infill microstructures are built within the geometry of the macroscale structural configuration. Using the commercial software COMSOL Multiphysics (COMSOL Multiphysics, [n.d.](#)), the macrostructure and microstructures are constructed based on the obtained optimization results. Then, with the repetition of microstructures, a boolean operation is conducted mix the structures at two scales into a single-scale structure. Finally, a body-fitted mesh composed of 2,405,090 triangular elements is created to describe geometrical characteristics in detail, as shown in the right half of Fig. 3.17. Subsequently, the two-dimensional finite element analysis of the model is performed.

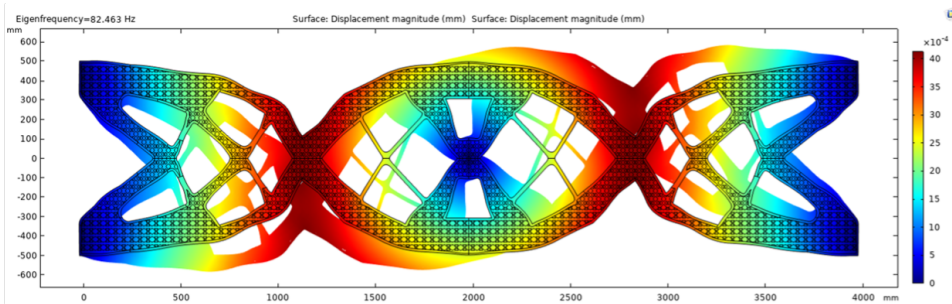
As can be observed in Fig. 3.18, there is no local vibration exists in the first three eigenmodes of the coated structure, even though there are many slender bars or truss-like structures with softer and lighter material properties in the macroscale structure. Table 3.2 labels eigenfrequencies computed using COMSOL (based on the structure shown in Fig. 3.17) and MATLAB (based on the structure shown in Fig. 3.15a), respectively. Although there exist about 10 % differences, values of the first three eigenfrequencies match well considering the huge difference between the mesh size in two models and different types of elements we utilized. The calculated dynamic compliance value of the structure is $1.17 \cdot 10^{-3} \text{N} \cdot \text{m}$, also yielding a roughly 12 % difference from the one calculated in MATLAB. This analysis result reveals that the energy-based homogenization method and the finite element analysis in the code we developed are both reliable.



(A)



(B)



(C)

FIGURE 3.18: Eigenmode shapes of the optimized clamped ends beam: (a) 1st, (b) 2nd, and (c) 3rd eigenmodes.

3.6 Summary

This paper has proposed an efficient multiscale topology optimization framework to minimize the dynamic compliance of coated structures by designing layer-wise bi-material lattice infilling. In this method, coated structures are covered by an outer coating of uniform thickness and the substrate areas of them are uniformly (or near-uniformly) divided into several layers. All layers are composed of the periodic distribution of multiple patterns of bi-material microstructures. The VFLS method is utilized to perform macroscale structural design, and structural boundaries with great smoothness can be obtained. With the help of the signed distance property, only two level set surfaces of one single level set function are needed to clearly model the different structural regions. In addition, the thickness of the coating can be well maintained during the iteration. For multi-layer lattice infilling, various topological configurations of bi-material microstructures are optimized using the popular SIMP method. The energy-based homogenization method is applied to evaluate the homogenized elasticity tensor of microstructures, which bridges the different scales. Generally, the proposed multiscale topological design approach combines the great advantages of the VFLS method and the SIMP method. In particular, different types of design variables at two scales are updated simultaneously in the proposed research thanks to the VFLS method's ability of implementing general mathematical programming algorithms. According to the numerical examples, several remarkable features of the proposed method can be obtained. Firstly, designing layer-wise bi-material lattice infill can lead to coated structures with lower dynamic compliance than those infilled with traditionally periodic and uniform lattice microstructures. Second, the number of divided layers has a great influence on the topologies of optimized structures at scales, and the division direction for the bi-material lattice infill microstructures should be carefully considered for a better performance of optimization results. Third, new macroscale geometrical features will emerge by changing the damping coefficients, while the microstructural configurations may remain the same. Also, different static constraints and different excitation frequencies can lead to varied macrostructures but may have little influence towards optimized microstructural configurations using the developed approach. When an excitation frequency higher than the fundamental eigenfrequency is considered, a relatively lower dynamic compliance can be achieved with a larger allowed value on the static compliance. Besides, using the proposed approach, different macrostructural configurations and microstructures can be obtain with variation of the thickness of the outer coating. Next, low mesh-dependency performance has been observed for the proposed method, but much finer geometrical features can be generated by using finer element meshes at two scales. Finally, the finite element analysis results using the body-fitted mesh match well with the one calculated using the proposed framework and thus the effectiveness of the developed concurrent multiscale topological design strategy is well verified.

Chapter 4

Multimaterial topology optimization of coated structures[†]

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4.1 Introduction

Coated structures are widely existed in the natural kingdom, such as cortical bone, bamboo, bird beak, and plant stems. Also known as shell-infill structures, such bio-inspired structures are usually made of a solid external coating and an internal substrate or porous infilling (Wu, Aage, Westermann, and Sigmund, 2017; Wadbro and Niu, 2019; Hu, Wang, Zhang, Li, Ding, Izui, and

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Nishiwaki, 2022). Functionally, the external coating can offer a protection to the substrate of structures and further improve certain structural performance (like a higher stiffness-to-weight ratio (Gibson, 2003) or a better buckling resistance ability (Clausen, Aage, and Sigmund, 2016; Thomsen, Wang, and Sigmund, 2018)) with the combination of the merits of different materials. Till now, coated structures have attracted great attention from industry to academia and exhibited great potential in various applications, including vibration mitigation (Matlack, Bauhofer, Krödel, Palermo, and Daraio, 2016), energy absorption (Tancogne-Dejean, Spierings, and Mohr, 2016), and medical implant (Nickels, 2012a).

As a branch of structural optimization, topology optimization (TO) owns much larger design freedom compared to size optimization and shape optimization, being widely regarded as an effective and powerful tool to design advanced structures due to its great ability in determining the optimized material distribution for concerned structural functionalities. Many attractive topology optimization approaches have been proposed during the past few decades. Among them, solid isotropic material with penalization (SIMP) method (Bendsøe and Sigmund, 1999; Sigmund, 2001), evolutionary structural optimization (ESO)/ bi-directional ESO (BESO) method (Xie and Steven, 1993; Huang, Xie, and Burry, 2006), level set (LS) method (Gao, Luo, Li, and Gao, 2019; Wang, Wang, and Guo, 2003; Wang and Kang, 2018b), and moving morphable components/voids (MMC/MMV) method (Zhang, Yuan, Zhang, and Guo, 2016; Zhang, Li, Yuan, Song, and Guo, 2017) are the most popular optimization methods. With vigorous research activities, topology optimization has been successfully applied to diverse optimum design problems, including reinforcement optimization (Hu, Ding, Shen, and Zhang, 2020; Shen, Ding, Hu, Zhang, and Xu, 2021; Hu, Ding, Zhang, Shen, and Li, 2023), bionic design (Li, Yu, Jolivet, Alexandersen, Kondoh, Hu, Furuta, Izui, and Nishiwaki, 2023; Zhao, Zhao, Ma, Wu, Yang, and Feng, 2015), thermal cloaking (Xu, Gu, and Chen, 2023; Wang, Sha, Xiao, Qiu, and Gao, 2023), composite material design (Zhang, Takezawa, Ding, Guo, Ni, and Zhang, 2021; Hu, Luo, and Liu, 2021; Jia, Luo, Takezawa, and Zhang, 2022), etc.

Since the pioneering research work of Clausen et al. (Clausen, Aage, and Sigmund, 2015), designing coated structures via the topology optimization technique is getting more and more attention in the optimization community. However, a critical issue arises in the design of coated structures regarding how to distinguish the external coating and the internal substrate region during the optimization process. When dealing with this issue, LS methods exhibit their great advantages that the external coating with uniform thickness can be easily and directly described by the contour lines of a LS surface due to the signed distance properties. Therefore, lots of research work on the topology optimization of coated structures are based on LS methods. For instance, Wang and Kang (Wang and Kang, 2018a) firstly proposed a LS-based topology optimization approach for the design of 2D and 3D coated structures. Fu et al. (Fu, Li, Xiao, Gao, and Chu, 2019) addressed coated structure design by using a new parametric LS (PLS) method, in which the PLS function is regularized to a signed distance function with an introduced distance regularization term. Then, this regularized PLS approach was also extended to the design of coated structures

infilled with microstructures (Fu, Li, Gao, and Xiao, 2019). In the research of Jiang et al. (Jiang, Guo, Chen, Wei, Lei, and Gu, 2019), a new type of cardinal basis functions is constructed and introduced into the PLS method for the design of coated structures, with which the bounds of design variables are able to be considered within the optimizer. Some researchers use geometric components to optimize coated structures. For example, Hoang et al. (Hoang, Tran, Nguyen, Hackl, and Nguyen-Xuan, 2020) designed coated structures by employing an adaptive mapping technique of adaptive geometric components, which are sandwich bars composed of a solid coating and the porous infill. In the research of Liu et al. (Liu, Du, Zhu, Zhang, Zhang, and Guo, 2020), a hybrid MMC-MMV method was proposed for the topology optimization of coated structures with graded infilling, in which the coating is searched with the help of topology description functions. Different from other methods, special schemes (generally filtering and projection operations) are needed for density-based methods to find the distribution of the external coating and the substrate region among the density field. Typically, a two-step filtering and interpolation approach was proposed in the research of Clausen et al. (Clausen, Aage, and Sigmund, 2015; Wu, Clausen, and Sigmund, 2017) to identify material interfaces, which involves the calculation of the spatial gradient of a smoothed density field. Based on the previous work, Groen et al. (Groen, Wu, and Sigmund, 2019) further developed a successive smoothing projection and gradient operations to solve the coating indication. Similarly, Zhou et al. (Zhou, Lu, Liu, and Lin, 2022; Liu, Zhou, Wei, and Lin, 2021) optimized coated structures with self-supported infilling. Without calculating the spatial gradient of the density field, Yoon and Yi (Yoon and Yi, 2019) established a new density filter by multiplying the modified densities and the original densities to find the coating during the optimization and the thickness of the coating is controlled via a radius parameter. Subsequently, Yi et al. (Yi, Yoon, and Peng, 2021) improved the procedure in (Yoon and Yi, 2019) and identified the coating based on the smoothed and projected density fields. Høghøj et al. (Høghøj, Nørhave, Alexandersen, Sigmund, and Andreasen, 2020) identified the domains of two fluids and their interfaces with an erosion-dilation technique and optimized the topology of two fluid heat exchangers. Luo et al. (Luo, Li, and Liu, 2019) developed an erosion-based interface identification approach for the topology optimization of coated structures. Then, they extended this method to multiscale topology optimization problem by identifying the interfaces of different microstructural areas (Luo, Hu, and Liu, 2021). In the recent research work of Postigo et al. (Postigo, Garaigordobil, Ansola, and Canales, 2024), a novel filtering scheme is proposed to design coated structures, in which the coating thickness is explicitly achieved by employing the SUSAN (Smallest Univalued Segment Assimilating Nucleus) algorithm to find the structural contour and the Robin boundary condition is introduced for the smoothing.

Recently, another increasingly popular topic in the field of topology optimization is designing structures consist of multi-phase materials. Different from those commonly designed single-material structures, structures with a reasonable distribution of different materials may show advantages in weight/cost reduction while maintaining a satisfactory structural performance or achieve certain purposes (Sigmund and Torquato, 1997; Nguyen, Tran, Nguyen, and Bui, 2023). To optimize multi-material structures under the LS framework, Wang and Wang (Wang and Wang,

2004) developed a “color” LS (CLS) method in which m number of LS functions are used to represent 2^m materials. Then, this method was successively applied to design multi-material compliant mechanisms (Wang, Chen, Wang, and Mei, 2005). Wang et al. (Wang, Luo, Kang, and Zhang, 2015) proposed a multi-material LS (MMLS) topology description model to optimize multi-phase structures, which used totally m LS functions for the description of $(m+1)$ phases. Noda et al. (Noda, Noguchi, and Yamada, 2022) and Nakayama et al. (Nakayama, Li, Furuta, Izui, and Nishiwaki, 2023) introduced multiple LS functions into their reaction-diffusion-equation-driven multi-material topology optimization. Under the SIMP framework, Sigmund and Torquato (Sigmund and Torquato, 1997) established a mixture model of three-phase material interpolation scheme for multi-material structures. Subsequently, Bendsøe and Sigmund (Bendsøe and Sigmund, 1999) designed two-material structures with different design variables using several interpolation schemes. Yin and Ananthasuresh (Yin and Ananthasuresh, 2001) developed a peak function material interpolation model, in which only one design variable is used for the description of varied materials. Focused on mass constraint problems, Gao and Zhang (Gao and Zhang, 2011) tested the effectiveness of recursive multi-phase materials interpolation (RMMI) and uniform materials interpolation (UMMI) schemes in multi-material topology optimization, respectively. Wu et al. (Wu, Fang, and Li, 2019) addressed the multi-material topology optimization of thermomechanical structures with the employment of the rational approximation of material properties (RAMP) model and the buckling resistance ability was enhanced. Majdi and Reza (Majdi and Reza, 2020) adopted the SIMP method and alternating active phase algorithm (Tavakoli and Mohseni, 2014) into the multi-material compliant mechanism design. Varied from the above density methods, Zuo and Saitou (Zuo and Saitou, 2017) constructed a novel ordered SIMP interpolation scheme to design multi-material structures. In this scheme, candidate materials are represented by the ordered normalized densities without the introduction of additional design variables. Then, Xu et al. (Xu, Liu, Zou, Li, and Ma, 2021) utilized the ordered SIMP approach to solve stress-constrained multi-material topology optimization problems. Zhang et al. (Zhang, Xiao, Li, Gao, and Chu, 2018) optimized the macro-scale multi-material distribution of composite structures via the ordered SIMP method. Based on the BESO method, Gan et al. (Gan and Wang, 2021) employed the polynomial interpolation scheme for design variable description of multi-material structures considering static and dynamic characteristics. Apart from LS-based and density-based methods, Zhang et al. (Zhang, Song, Zhou, Du, Zhu, Sun, and Guo, 2018) established a new MMC-based multi-material topology optimization framework. Additionally, using iso-geometric analysis (Gao, Wu, Xiao, Nguyen, Gao, and Rabczuk, 2023), multi-phase material description models are constructed by Yang et al. (Yang, Wang, Luo, Xie, and Xiong, 2022) and Lieu et al. (Lieu and Lee, 2017), respectively.

Combining the advantages of coated structures and multi-material structures, a few researchers have also conducted topology optimization of coated structures with multiple infill materials. As an example, Bai and Zuo et al. (Bai and Zuo, 2022) employed the MMLS approach to seek the multi-material optimal layout within coated structures, where only the signed distance property

of the LS surface which distinguished the solid and the void parts is utilized for the coating identification. However, to the best knowledge of the authors, only LS methods and few density-based methods have been successfully applied to design the topology of coated structures infilled with multiple materials so far. Although the optimized multi-microstructural composite structures are coated using an improved ordered SIMP method in the research of Gu et al. (Gu, He, Dong, and Song, 2022), there is not only a solid outer coating but also several solid interface layers within the structures they designed to connect several types of optimized microstructures. Thus, it is not counted into the “true” multi-material structures covered by an outer coating (which we plan to design) in this research and the corresponding density-based research still needs to be developed.

With these circumstances and aspiration to further moves a step, a novel ordered SIMP-based topology optimization method is constructed in this paper to design coated structures infilled with multiple materials. Specially, a new material interpolation scheme consists of several filtering and projection operations is proposed to separate the coating and identify the multi-phase material layout for the substrate based on the design variable field. To be specific, two special Heaviside projections, i.e., a piece-wise Heaviside projection and a “strict” Heaviside projection, are introduced into the classical two-step filtering identification process and a new material modeling scheme is developed. After identifying the coating and the substrate area based on filtered design variables, the infilling with optimized layout of multiple materials can be obtained by multiplying the piece-wise projected density field and the infilling identification density field. With the growth of iteration step and corresponding parameters, distribution of the coating and the multiple infill materials is gradually stabilized. In this way, the outer coating and the multi-material infilling can be simultaneously optimized and the interaction effect between them is explicitly considered during the optimization. Inheriting the advantages of the ordered SIMP approach, neither pre-processing of the design domain nor additional design variables are needed in the proposed method, resulting in a great structural performance while saving the computational cost. In addition, numerical tests reveal that the proposed new material interpolation scheme has the ability to generate results with great structural performance with variation of corresponding design parameters.

The reminder of this paper is organized as follows. In Section 4.2, the material modeling scheme relied on the new filtering and projection process is proposed. Section 4.3 constructs formulations for the topology optimization problem and the optimization procedure is introduced. Section 4.4 derives the sensitivity analysis and several numerical examples are provided in Section 4.5 to illustrate the effectiveness of the proposed method. Finally, conclusions are presented in Section 4.6.

4.2 A new material interpolation scheme for coated structures with multi-material infilling

4.2.1 General idea

Taking a bi-material infilling as an example, the general idea of the identification of the external coating and the inner multi-material distribution is presented in Fig. 4.1. To begin with, the bi-material structure (depicted using two densities, i.e., 0.5 and 1.0) shown in Fig. 4.1(a) is projected to obtain a solid structure as shown in Fig. 4.1(b). Next, this solid structure is further eroded and yields an eroded structure presented in Fig. 4.1(c). As presented in Fig. 4.1(d) with the desired thickness, the external coating of the structure can be defined by the different parts between the solid structure and its eroded structure. Finally, the expected coated structure with multiple material infilling can be obtained with the combination of the original structure given in Fig. 4.1(a) and the external coating presented in Fig. 4.1(d).

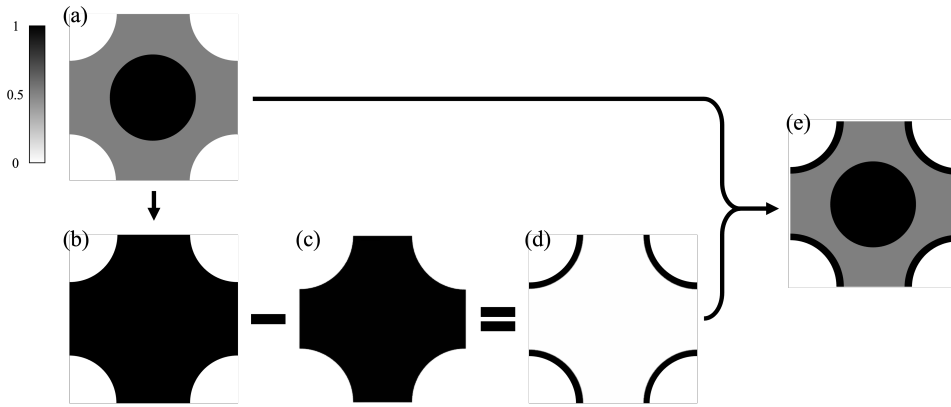


FIGURE 4.1: General idea for the identification of the external coating and the construction of a coated structure with multi-material infilling. (a) The original multi-material structure; (b) The solid structure; (c) The eroded structure; (d) The external coating; (e) The coated structure infilled with multiple materials.

It should be emphasized that three critical issues exist during this procedure. First, the projection from the original multi-material structure to the solid structure should be precise enough to distinguish whether there is material or not, regardless of possible intermediate densities. Second, all the materials considered for the substrate should be covered by the external coating. Third, the thickness of the external coating should be an expected value, requiring an explicit or implicit relationship with corresponding projection or erosion parameters.

4.2.2 Heaviside projection

Standard Heaviside projection

In those density-based topology optimization approaches, the following standard continuous Heaviside projection (Wang, Lazarov, and Sigmund, 2011) is usually selected to obtain clear black-/white designs based on the tangent function. In the proposed topology optimization method for coated structures infilled with multiple materials, this standard Heaviside projection is utilized for the external coating identification.

$$\bar{x} = \frac{\tanh(\beta_h \eta_h) + \tanh(\beta_h (x - \eta_h))}{\tanh(\beta_h \eta_h) + \tanh(\beta_h (1 - \eta_h))}, \quad (4.1)$$

where x and $\bar{x}$ are density fields before and after the standard continuous projection; β_h is a parameter to control the "sharpness" of the standard Heaviside projection and the notion η_h denotes the threshold value for the projection. The standard Heaviside projection Eq. (4.1) works as a true Heaviside step function when the sharpness parameter β_h approaches infinity.

Piece-wise Heaviside projection

In the classical ordered SIMP approach developed by Zuo and Saitou (Zuo and Saitou, 2017), multiple materials are described by certain densities which are arranged in the ascending order of the normalized design variable ρ_i^A and each normalized density corresponding to one type of materials. The normalized density can be formulated as

$$\rho_i^N = \rho_i^A / \rho_{\max}, \quad i = 1, 2, 3, \dots, m, \quad (4.2)$$

where $\rho_{\max}$ is the maximum density among all of the candidate densities and m is the total number of materials considered. It should be noted that the void elements are also regarded as a material with an extremely low density value. In this paper, the minimum normalized density is set as $\rho_1^N = 10^{-6}$ to avoid singular matrices.

To obtain clear multi-material layout with the description of the normalized densities ρ_i^N , a continuous piece-wise Heaviside projection is obtained with ρ_i^N based on the standard Heaviside projection (Gu, He, Dong, and Song, 2022). For design variable $\rho_e \in [\rho_i^N, \rho_{i+1}^N]$, the projection is formulated as

$$\hat{\rho}_e = \left(\rho_{i+1}^N - \rho_i^N \right) \frac{\tanh(\beta_p \eta_p) + \tanh(\beta_p (\rho_e - \eta_p))}{\tanh(\beta_p \eta_p) + \tanh(\beta_p (1 - \eta_p))} + \rho_i^N, \quad i = 1, 2, \dots, m-1, \quad e = 1, 2, \dots, n, \quad (4.3)$$

$$\rho_A = \frac{\rho_e - \rho_i^N}{\rho_{i+1}^N - \rho_i^N}, \quad i = 1, 2, \dots, m-1, \quad e = 1, 2, \dots, n, \quad (4.4)$$

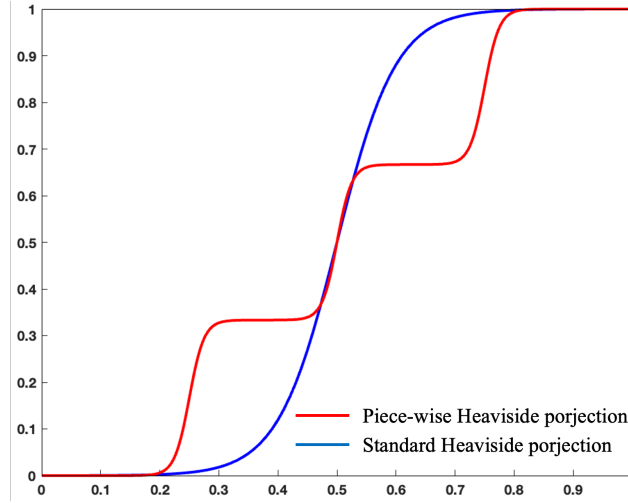


FIGURE 4.2: Comparison of the projection effect between the standard and the piece-wise Heaviside projections.

where $\hat{\rho}_e$ is the projected element density through the piece-wise Heaviside projection; β_p and η_p are the sharpness parameter and the threshold parameter, respectively; n denotes the total number of design variables. The difference between the standard and the piece-wise Heaviside projections is shown in Fig. 4.2. Actually, the continuous piece-wise Heaviside projection Eq. (4.3) can be regarded as performing the standard continuous Heaviside projection Eq. (4.1) in each density interval, which projects the intermediate densities within the interval to the normalized density ρ_i^N or ρ_{i+1}^N , resulting a clear multi-material presentation.

Strict Heaviside projection

Different from those existing research for coated structure design, a strict Heaviside projection is developed into the proposed topology optimization method, which is critical for the identification of the external coating for multi-material structures. Theoretically, it has no difference from the above standard Heaviside projection Eq. (4.1) but the threshold value η_s is comparatively smaller to correctly define the substrate region for multi-phase infill materials. An illustration is presented in Fig. 4.3 for a better understanding. After the piece-wise Heaviside projection with a non-infinity β_p value, the design domain presented in Fig. 4.3(a) contains densities range from ρ_1^N to 1, describing the layout of three infilling materials. With the strict Heaviside projection, a density field contains obvious void/solid material distribution is obtained, as illustrated in Fig. 4.3(b). It can be observed that this density field covers all the regions that have infilling materials ($\rho > \rho_1^N$) shown in Fig. 4.3(a) and it is used for the following steps to further identify the external coating and the substrate region of coated structures.

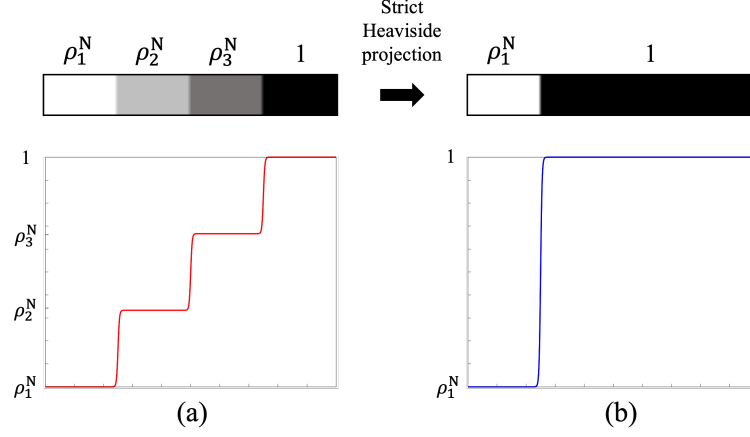


FIGURE 4.3: Illustration of the effect of the strict Heaviside projection.

4.2.3 PDE-based filter

After obtaining the strictly projected density field ρ_s , a two-step filtering and projection will be implemented for the identification of the external coating and the internal multi-material substrate. A commonly used PDE (Partial Differential Equation) filter based on a Helmholtz-type partial differential equation (Lazarov and Sigmund, 2011) is selected to conduct the filtering, with a filtering formula constructed as

$$-r^2 \nabla^2 \tilde{\mathbf{X}} + \tilde{\mathbf{X}} = \mathbf{X}, \quad (4.5)$$

where $\mathbf{X}$ and $\tilde{\mathbf{X}}$ denote the density fields before and after the filtering operation, respectively; r is a length scale parameter, whose value can be determined by a filter radius R using the following equation:

$$r = \frac{R}{2\sqrt{3}}. \quad (4.6)$$

4.2.4 Material interpolation scheme

The overall process of the newly proposed filtering and projection procedure for the design of coated structures infilled with multi-phase materials is presented in Fig. 4.4, with all control parameters labeled on. Generally, the whole procedure is composed of three stages.

During the first stage, the original density field ρ containing various densities is firstly piecewisely projected into a density field $\hat{\rho}$ based on Eq. (4.3), with control parameters β_M and $\eta_M = 0.5$. Under the framework of the ordered SIMP method, the elastic modulus and the mass of multiple materials in the density field $\hat{\rho}$ are respectively formulated as

$$E(\rho_e) = A_E \rho_e^p + B_E, \quad e = 1, 2, \dots, n, \quad (4.7)$$

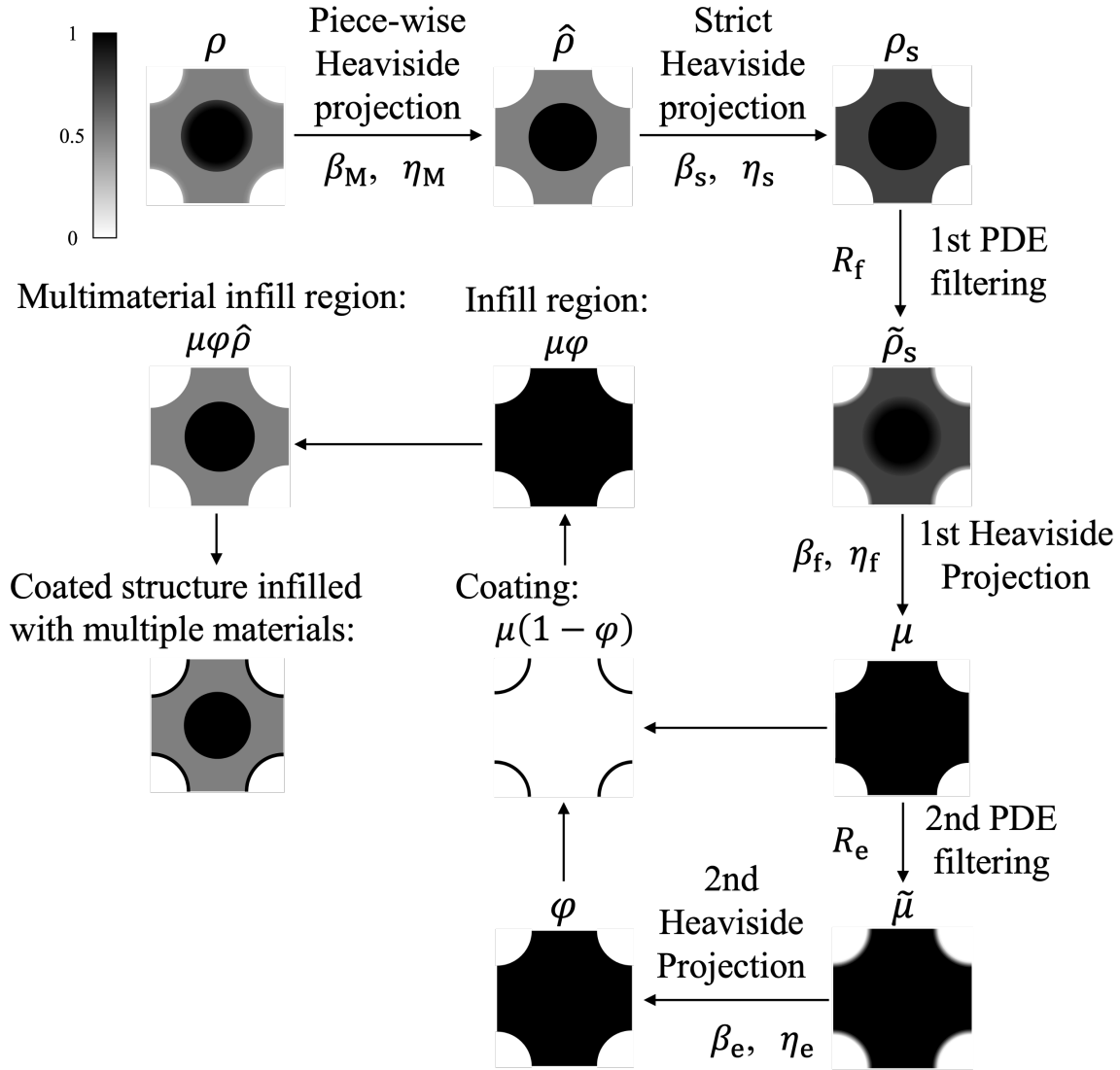


FIGURE 4.4: A new filtering and projection process for the modeling of coated structure infilled with multiple materials.

$$M(\rho_e) = A_M \rho_e^p + B_M, \quad e = 1, 2, \dots, n, \quad (4.8)$$

where p is the penalization factor; A_E , A_M are the scaling coefficients and B_E , B_M are the translation coefficients, respectively. For $\rho_e \in [\rho_i^N, \rho_{i+1}^N]$, A_E , A_M , B_E , and B_M are respectively defined as

$$A_E = \frac{E_i - E_{i+1}}{(\rho_i^N)^p - (\rho_{i+1}^N)^p}, \quad i = 1, 2, \dots, m-1, \quad (4.9)$$

$$A_M = \frac{M_i - M_{i+1}}{(\rho_i^N)^p - (\rho_{i+1}^N)^p}, \quad i = 1, 2, \dots, m-1, \quad (4.10)$$

$$B_E = E_i - A_E (\rho_i^N)^p, \quad i = 1, 2, \dots, m-1, \quad (4.11)$$

$$B_M = M_i - A_M (\rho_i^N)^p, \quad i = 1, 2, \dots, m-1, \quad (4.12)$$

where E_i and E_{i+1} , M_i and M_{i+1} are the elastic modulus and the mass of the ordered material i and $i+1$, respectively.

Then, using the strict Heaviside projection, the density field ρ_s is further projected into a base density field ρ_s , which is used for the following coating identification. In order to successfully detect all the regions of having non-void materials in the density field $\hat{\rho}$, the threshold parameter η_s is set as $\eta_s = \rho_2^N - \varepsilon$ with a pretty small non-zero parameter ε (e.g., $\varepsilon = 10^{-3}$). It should be noted that the information of multiple material layout within the design domain is eliminated after this step and it has no influence on the coating identification.

Next, the classical two-step filtering and projection is conducted to distinguish the coating and the substrate region, which can successfully prevent the checkerboard design or gray structural boundaries (Luo, Li, and Liu, 2019). After obtaining the density field μ with the first filtering and projection, an erosion is performed with a relatively larger threshold value $\eta_e = 0.5 + \Delta\eta_e$. With a simple algebraic formation, the different and shared parts between the smoothed density field μ and its eroded density field ϕ determine the external coating and the substrate, respectively. To be specific, the coating is modeled by $\mu = 1$ and $\phi = 0$, and the substrate region is determined by $\mu = \phi = 1$. It should be noted that the coating identification scheme used in the proposed study has no difference with those relying on eroded and dilated structures. However, the optimization of multiple material layout within coated structures cannot be achieved using those methods based on one design variable field, and this issue has been considered in the method we developed.

The elastic modulus and mass formulas of the structure can be written as (Luo, Li, and Liu, 2019; Yi, Yoon, and Peng, 2021)

$$E(\mu, \phi, \hat{\rho}) = \mu^p [\phi^p E_{\text{substrate}} + (1 - \phi^p) E_{\text{coating}}], \quad (4.13)$$

$$M(\mu, \phi, \hat{\rho}) = \mu [\phi M_{\text{substrate}} + (1 - \phi) M_{\text{coating}}], \quad (4.14)$$

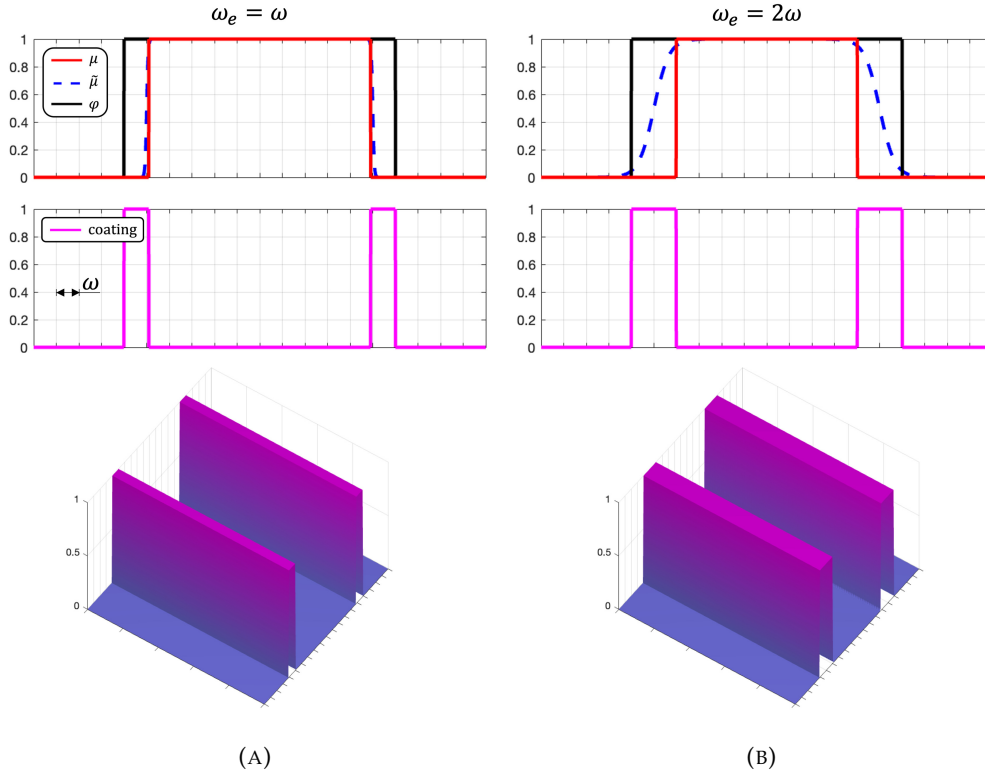


FIGURE 4.5: Illustration of coating thickness from changing the ω_e parameter from ω (left) to 2ω (right).

where $E_{\text{substrate}}$ and $M_{\text{substrate}}$ denote the elastic modulus and mass of the substrate region, respectively; E_{coating} and M_{coating} are the elastic modulus and mass of the coating, respectively. When $\Delta\eta_e$ is given as 0.45, the thickness of the coating ω_e can be achieved by the radius filter R_e for the second filtering operation as

$$\omega_e \approx 1.5R_e. \quad (4.15)$$

Analytical details of the above equation can be referred to the research work of Luo et al. (Luo, Li, and Liu, 2019). For a better understanding, an illustration on achieving different coating thicknesses is presented in Fig. 4.5, in which two cases of coating thicknesses are considered.

Eventually, the multi-phase material distribution within the substrate can be identified by multiplying the piece-wisely projected density field $\hat{\rho}$ with the infill region indication field $\mu\phi$. Therefore, the $E_{\text{substrate}}$ and $M_{\text{substrate}}$ introduced in Eq. (4.13) and Eq. (4.14) can be formulated as

$$E_{\text{substrate}} = A_E \hat{\rho}^p + B_E. \quad (4.16)$$

$$M_{\text{substrate}} = A_M \hat{\rho}^p + B_M. \quad (4.17)$$

As a result, the final elastic modulus and mass functions can be further given as

$$E(\mu, \varphi, \hat{\rho}) = \mu^p [\varphi^p (A_E \hat{\rho}^p + B_E) + (1 - \varphi^p) E_{\text{coating}}] . \quad (4.18)$$

$$M(\mu, \varphi, \hat{\rho}) = \mu [\varphi (A_M \hat{\rho}^p + B_M) + (1 - \varphi) M_{\text{coating}}] . \quad (4.19)$$

With the combination of the coating identified during the second stage, the newly defined multi-material infilling can be covered by an external coating and finally an ideal coated structure is obtained.

It should be noted that the coating separation starts from the first iteration step but no clear coating can be achieved at early steps. In fact, a clear coating is not expected to be generated during the early optimization process because a premature coating will definitely affect the optimization of the coated structure, leading to a result of inferior structural performance. Therefore, the PDE filtering and the Heaviside projections we initially applied on the design variable field are pretty weak, with a highly vague coating identified. When the iteration step increases, corresponding parameters gradually become larger with stronger projection effects, and then the coating separation can be slowly achieved with the growth of the structural configuration. In this way, the design freedom of the TO process is ensured and the coated structure can be successfully designed with a clear coating presented.

Compared to those existing filtering schemes for the coating identification, the proposed new filtering and projection procedure has the ability to describe the external coating and its inner multi-material layout. Besides, it's easy to implement because all the key techniques in the new scheme are based on those commonly-used PDE filtering and continuous Heaviside projections.

4.3 Topology optimization of coated structures with multiple infill materials

4.3.1 Problem formulation

In this research, the static compliance minimization problem is considered with a mass constraint for the limitation of multi-material layout within coated structures. The mathematical model can be constructed as

$$\begin{aligned} \min : & c(E(\mu, \varphi, \hat{\rho})), \\ \text{s.t. } & \mathbf{K}(E(\mu, \varphi, \hat{\rho})) \cdot \mathbf{U}(E(\mu, \varphi, \hat{\rho})) = \mathbf{F}, \\ & G = \sum_{e=1}^n M_e(\mu, \varphi, \hat{\rho}) - M_f \cdot M_{\text{ref}} \leq 0, \\ & \mu_e, \varphi_e \in [0, 1], \quad e = 1, 2, \dots, n, \end{aligned} \quad (4.20)$$

where c is the static compliance of the structure; $E(\boldsymbol{\mu}, \boldsymbol{\varphi}, \hat{\boldsymbol{\rho}})$ and $M(\boldsymbol{\mu}, \boldsymbol{\varphi}, \hat{\boldsymbol{\rho}})$ are the interpolated elastic modulus and mass fields, respectively; $\mathbf{K}$ is the global stiffness matrix and $\mathbf{U}$ is the global displacement of the structure; $\mathbf{F}$ represents the external load vector; G denotes the mass constraint and M_f is the maximum allowed mass fraction; M_{ref} is the mass of a reference structure and it equals to the one of the design domain filled with a certain material. In particular, Bai and Zuo (Bai and Zuo, 2022) compared the effectiveness of the total mass constraint and multiple volume constraints and found both of them can generate reasonable structural configurations of coated structures. Thus, to effectively control the consumption of all considered materials with only one constraint, the mass constraint is used in this study as other research works (Yi, Yoon, and Peng, 2021; Sivapuram, Picelli, Yoon, and Yi, 2021).

The calculation of the global stiffness matrix is based on the following equation:

$$\mathbf{K} = \sum_e^n E_e(\boldsymbol{\mu}, \boldsymbol{\varphi}, \hat{\boldsymbol{\rho}}) \mathbf{k}^0, \quad (4.21)$$

where $\mathbf{k}^0$ is the stiffness matrix of an element with unit Young's modulus and can be expressed using the Poisson's ratio ν as follows:

$$\mathbf{k}^0 = \frac{1}{1 - \nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix}. \quad (4.22)$$

During the optimization, the mass constraint has to be updated because it is not directly imposed on the intermediate design and may cause an offset of the final structural mass from the prescribed maximum mass value (Luo, Li, and Liu, 2019). The mass fraction M_f^* used to evaluate the constraint at each iteration step is updated using the following equation:

$$M_f^* = \frac{M^*}{M^{i'}} M_f, \quad (4.23)$$

where M^* and $M^{i'}$ are the prescribed maximum mass and the mass of the structure at the i' -th iteration step, respectively.

4.3.2 Optimization procedure

The flowchart for solving the topology optimization of coated structures with multiple infill materials using the proposed new filtering and projection scheme is illustrated in Fig. 4.6, and the detailed explanation is given as follows:

1. Initialize the structure and define the boundary conditions for the FE analysis and design.

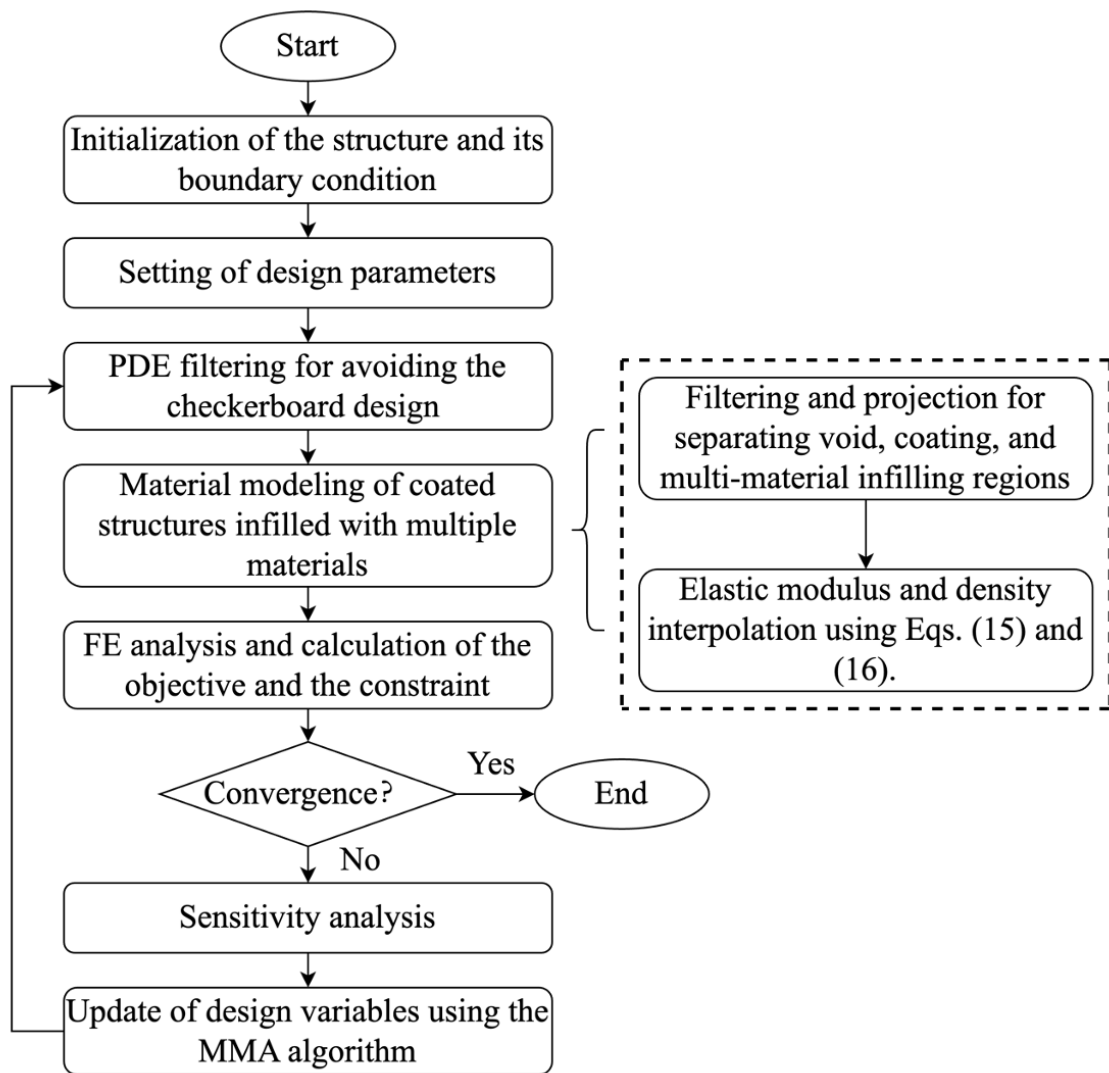


FIGURE 4.6: Flowchart illustrating the topology optimization process for coated structures infilled with multiple materials.

2. Set all the design parameters in the proposed procedure. The thickness of the external coating ω_e is achieved by the parameters R_e and $\Delta\eta_e$, using Eq. (4.15) during the classical two-step filtering and projection.
3. Carry out the PDE filtering for avoiding the checkerboard design.
4. Construct the model of coated structures with multiple infill materials, including the separation of void, coating, and multi-material infilling regions, and interpolate the elastic modulus and density using filtered or projected intermediate density fields.
5. Implement FE analysis and compute the objective and constraint.
6. Check whether the convergence condition is satisfied. If it's satisfied, the optimization is finished and the final optimized coated structure is obtained; If not, continue to Step (7).
7. Calculate the sensitivity and update design variables using the Method of Moving Asymptotes (MMA) (Svanberg, 1987) algorithm.
8. Return back to Step (3) and repeat the procedure.

4.4 Sensitivity calculation

Using the self-adjoint property of the problem, the first-order derivative of the static compliance with respect to the design variables can be written as

$$\frac{\partial c}{\partial \rho_e} = -\mathbf{U}^T \frac{\partial \mathbf{K}}{\partial \rho_e} \mathbf{U} = -\sum_i^n \frac{\partial E_i}{\partial \rho_e} (\mathbf{u}_i^T \mathbf{k}^0 \mathbf{u}_i). \quad (4.24)$$

Based on Eq. (4.18), the term $\partial E_i / \partial \rho_e$ in the above equation can be formulated using the product rule as

$$\begin{aligned} \frac{\partial E_i}{\partial \rho_e} = & p \cdot \mu_i^{p-1} \frac{\partial \mu_i}{\partial \rho_e} [\varphi_i^p (A_E \cdot \hat{\rho}_i^p + B_E) + (1 - \varphi_i^p) E_{\text{coating}}] \\ & + \mu_i^p \left[p \cdot \varphi_i^{p-1} A_E \cdot \hat{\rho}_i^p \frac{\partial \varphi_i}{\partial \rho_e} + \varphi_i^p A_E \cdot p \cdot \hat{\rho}_i^{p-1} \frac{\partial \hat{\rho}_i}{\partial \rho_e} + p \cdot \varphi_i^{p-1} \frac{\partial \varphi_i}{\partial \rho_e} B_E - p \cdot \varphi_i^{p-1} \frac{\partial \varphi_i}{\partial \rho_e} E_{\text{coating}} \right]. \end{aligned} \quad (4.25)$$

Then, we rewrite the above Eq. (4.25) in a more clear expression as

$$\begin{aligned} \frac{\partial E_i}{\partial \rho_e} = & p \cdot \mu_i^{p-1} [\varphi_i^p (A_E \cdot \hat{\rho}_i^p + B_E) + (1 - \varphi_i^p) E_{\text{coating}}] \frac{\partial \mu_i}{\partial \rho_e} \\ & + \left[\mu_i^p \cdot p \cdot \varphi_i^{p-1} \cdot A_E \cdot \hat{\rho}_i^p + p \cdot \varphi_i^{p-1} \cdot B_E - p \cdot \varphi_i^{p-1} \cdot E_{\text{coating}} \right] \frac{\partial \varphi_i}{\partial \rho_e} \\ & + \mu_i^p \cdot \varphi_i^p \cdot A_E \cdot p \cdot \hat{\rho}_i^{p-1} \frac{\partial \hat{\rho}_i}{\partial \rho_e}. \end{aligned} \quad (4.26)$$

Using the chain rule, the term $\partial\mu_i/\partial\rho_e$ can be derived as

$$\frac{\partial\mu_i}{\partial\rho_e} = \frac{\partial\mu_i}{\partial\tilde{\rho}_{s_i}} \frac{\partial\tilde{\rho}_{s_i}}{\partial\rho_{s_i}} \frac{\partial\rho_{s_i}}{\partial\hat{\rho}_i} \frac{\partial\hat{\rho}_i}{\partial\rho_e}. \quad (4.27)$$

Similarly, the partial derivation of the eroded field φ with respect to the design variable ρ in Eq. (4.25) can be formulated as

$$\frac{\partial\varphi_i}{\partial\rho_e} = \frac{\partial\varphi_i}{\partial\tilde{\mu}_i} \frac{\partial\tilde{\mu}_i}{\partial\mu_i} \frac{\partial\mu_i}{\partial\rho_e} = \frac{\partial\varphi_i}{\partial\tilde{\mu}_i} \frac{\partial\tilde{\mu}_i}{\partial\mu_i} \frac{\partial\mu_i}{\partial\tilde{\rho}_{s_i}} \frac{\partial\tilde{\rho}_{s_i}}{\partial\rho_{s_i}} \frac{\partial\rho_{s_i}}{\partial\hat{\rho}_i} \frac{\partial\hat{\rho}_i}{\partial\rho_e}. \quad (4.28)$$

With Eq. (4.27) and Eq. (4.28), we can rewrite Eq. (4.26) as the following equation:

$$\begin{aligned} \frac{\partial E_i}{\partial\rho_e} &= p \cdot \mu_i^{p-1} [\varphi_i^p (A_E \cdot \hat{\rho}_i^p + B_E) + (1 - \varphi_i^p) E_{\text{coating}}] \frac{\partial\mu_i}{\partial\tilde{\rho}_{s_i}} \frac{\partial\tilde{\rho}_{s_i}}{\partial\rho_{s_i}} \frac{\partial\rho_{s_i}}{\partial\hat{\rho}_i} \frac{\partial\hat{\rho}_i}{\partial\rho_e} \\ &+ \left[\mu_i^p \cdot p \cdot \varphi_i^{p-1} \cdot A_E \cdot \hat{\rho}_i^p + p \cdot \varphi_i^{p-1} \cdot B_E - p \cdot \varphi_i^{p-1} \cdot E_{\text{coating}} \right] \frac{\partial\varphi_i}{\partial\tilde{\mu}_i} \frac{\partial\tilde{\mu}_i}{\partial\mu_i} \frac{\partial\mu_i}{\partial\tilde{\rho}_{s_i}} \frac{\partial\tilde{\rho}_{s_i}}{\partial\rho_{s_i}} \frac{\partial\rho_{s_i}}{\partial\hat{\rho}_i} \frac{\partial\hat{\rho}_i}{\partial\rho_e} \\ &+ \mu_i^p \cdot \varphi_i^p \cdot A_E \cdot p \cdot \hat{\rho}_i^{p-1} \frac{\partial\hat{\rho}_i}{\partial\rho_e}. \end{aligned} \quad (4.29)$$

According to Eq. (4.1), the sensitivity of the smoothed density variable μ with respect to the filtered density field $\tilde{\rho}_s$ can be obtained as

$$\frac{\partial\mu_i}{\partial\tilde{\rho}_{s_i}} = \beta_f \frac{1 - \tanh^2(\beta_f(\tilde{\rho}_{s_i} - \eta_f))}{\tanh(\beta_f\eta_f) + \tanh(\beta_f(1 - \eta_f))}, \quad (4.30)$$

where β_f and η_f are the sharpness parameter and the threshold value for the 1st standard Heaviside projection, respectively.

Similarly, the sensitivity calculation of the eroded field ϕ with respect to the secondly filtered density field $\tilde{\mu}$ is elaborated as

$$\frac{\partial\varphi_i}{\partial\tilde{\mu}_i} = \beta_e \frac{1 - \tanh^2(\beta_e(\tilde{\mu}_i - \eta_e))}{\tanh(\beta_e\eta_e) + \tanh(\beta_e(1 - \eta_e))}, \quad (4.31)$$

where β_e and η_e are the corresponding parameters for the 2nd standard Heaviside projection, respectively.

Associated with the strict Heaviside projection, the term $\partial\rho_s/\partial\hat{\rho}$ in Eq. (4.29) can also be given in a similar form as

$$\frac{\partial\rho_{s_i}}{\partial\hat{\rho}_i} = \beta_s \frac{1 - \tanh^2(\beta_s(\hat{\rho}_i - \eta_s))}{\tanh(\beta_s\eta_s) + \tanh(\beta_s(1 - \eta_s))}, \quad (4.32)$$

where β_s is the sharpness parameter for the strict Heaviside projection.

The sensitivity equation of the piece-wise Heaviside projection Eq. (4.3) can be obtained as

$$\frac{\partial \hat{\rho}_i}{\partial \rho_e} = \beta_M \frac{1 - \tanh^2(\beta_M(\rho_e - \eta_M))}{\tanh(\beta_M \eta_M) + \tanh(\beta_M(1 - \eta_M))}. \quad (4.33)$$

Based on the above expressions, the sensitivity of the mass constraint can be calculated and similarly derived in an arranged format as

$$\begin{aligned} \frac{\partial G}{\partial \rho_e} &= \frac{\partial M_i}{\partial \rho_e} \\ &= [\varphi_i (A_M \cdot \hat{\rho}_i^p + B_M) + (1 - \varphi_i) M_{\text{coating}}] \frac{\partial \mu_i}{\partial \rho_e} + \mu_i \cdot \varphi_i \cdot A_M \cdot p \cdot \hat{\rho}_i^{p-1} \frac{\partial \hat{\rho}_i}{\partial \rho_e} \\ &\quad + [\mu_i (A_M \cdot \hat{\rho}_i^p + B_M) - \mu_i \cdot M_{\text{coating}}] \frac{\partial \varphi_i}{\partial \rho_e}. \end{aligned} \quad (4.34)$$

4.5 Numerical examples

In this section, several 2D and 3D numerical examples are provided to demonstrate the efficiency of the proposed method in the design of coated structures infilled with multi-phase materials, which cover different coating thicknesses, different design parameters, different material properties, different mass constraints, and different infill materials. The penalization factor is set as $p = 3$ for all numerical examples. Following the recommendation in the research of Zuo and Saitou (Zuo and Saitou, 2017), the density field ρ is initialized as the value of the mass fraction M_f . In order to improve the stability of the algorithm, the initial sharpness parameters β_M^0 , β_s^0 , β_f^0 , and β_e^0 are all set as 1 (with a pretty small projection effect) and will be gradually increased with their certain increments $\Delta\beta_M$, $\Delta\beta_s$, $\Delta\beta_f$, and $\Delta\beta_e$ to 100. The initial threshold value η_s^0 for the strict Heaviside projection is set as the same value as ρ_1^N and the maximum value of η_s is defined as $(\rho_2^N - \vartheta)$, where $\vartheta = 0.01$ is used for a much more accurate distinguishment considering the projection effect. To reduce the number of design parameters that need to be defined, relationships $\Delta\beta_s = \Delta\beta_M$ and $\Delta\beta_e = \Delta\beta_f$ are constructed. The corresponding threshold parameters in all examples are given as $\eta_M = 0.5$, $\eta_f = 0.5$, and $\Delta\eta_e = 0.45$. As for the PDE filtering, the filter radius R_f is set as $R_f = 10$ and the value of the parameter R_e is calculated using Eq. (4.15). To obtain a clear material distribution of coated structures, a minimum iteration number $I_{\min}$ is introduced to ensure all the design parameters reach their maximum values. Besides, it can ensure an effective calculation of the structural mass on the final optimized structure.

All numerical examples are studied using the open source platform FreeFEM++ (Hecht, 2012). To ensure the erosion thickness at the structural boundaries and keep the final designs within the design domains, an extended void domain is added to all the structure setups and the values of μ within this extended domain is forced to be 0. The optimization will be terminated if one of the following conditions is satisfied: (1) the relative difference between the adjoint two objection

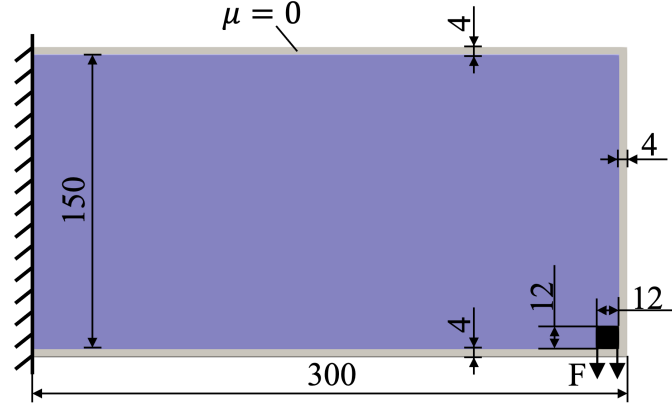


FIGURE 4.7: Design domain of the cantilever beam.

TABLE 4.1: Properties of the considered materials for the cantilever beam.

Name	Normalized density	Young's modulus	Mass	Color
Void	0	0	0	White
1	0.4	0.5	0.4	Green
2	1.0	1.0	1.0	Black

values is smaller than $1e-5$, with the iteration step larger than the given value $I_{\min}$; (2) the iteration reaches the predefined maximum number $I_{\max}$.

4.5.1 Cantilever beam

To begin with, we consider a typical cantilever beam structure, whose geometrical dimensions and boundary conditions are shown in Fig. 4.7. Two materials are considered in this example and their properties are listed in Table 4.1. Theoretically, the property of the infilling material is usually smaller than the one for the coating, but there is no difficulty in using the coating material as another candidate for the infilling because the same material can be used as the infilling material and to print the external coating using the AM technique. Therefore, the material 2 is selected for the construction of the coating and works as a candidate infilling material for the substrate. The allowed maximum mass fraction is set as $M_f = 50\%$. The minimum and the maximum iteration numbers are given as $I_{\min} = 100$ and $I_{\max} = 150$, respectively.

Different coating thicknesses

Firstly, three different thicknesses of the external coating are considered, i.e., $w_e = 2$, $w_e = 3$, and $w_e = 4$, leading to their radius parameters as $R_e = 3$, $R_e = 4.5$, and $R_e = 6$. Other design parameters that have not been defined are given as $\Delta\beta_M = 0.5$, $\Delta\eta_s = 0.01$, and $\Delta\beta_f = 1.0$. The

optimized cantilever beams are shown in Fig. 4.8 and they do include multiple infill materials and an external coating of uniform thickness. From amplified sub-figures, it can be seen that the coating thickness can be greatly controlled using the proposed scheme, proving the effectiveness of Eq. (4.15).

Generally, optimized cantilever beams shown in Fig. 4.8e share the same topology, which reveals that the thickness of the coating may have limited influence on the topology of optimization results. However, it can be seen that less material 2 is distributed among the substrate area of the structure presented in Fig. 4.8e than the other designs, since much more mass resource is allocated to the external coating in this case. Specially, the layout of the material 2 mainly concentrates near the fixed and the loading boundaries to better resist the structural deformation. The static compliance values of the optimized designs shown in Figs. 4.8a, 4.8c and 4.8e are $c = 6737.52$, $c = 6750.62$, and $c = 6762.28$, respectively. Different from the general consensus, a larger thickness of the external coating does not ensure a better structural performance in this research since it affects the distribution of the multiple infill materials under the mass constraint. Considering different coating thicknesses, iteration histories for the coated cantilever beam infilled with multiple materials are given in Fig. 4.8b, Fig. 4.8d, and Fig. 4.8f, respectively. In Fig. 4.8b, there is a significant increment on the compliance value which is because of the big change on the structural topology and can be eliminated by setting a smaller move step for MMA updating. Nevertheless, it can be observed that the proposed method has very stable iteration performance. Besides, the considered mass constraints for these cases of different thicknesses are all well satisfied and reach the specified maximum allowed values, proving the efficiency of the introduced mass update equation Eq. (4.23).

Effects of design parameters

In this subsection, effects of some design parameters used in the proposed method towards the final optimization results are tested, with the thickness of the coating defined as $w_e = 2$. Among all design parameters, there are five parameters that should be considered here, i.e., $\Delta\beta_s$, $\Delta\beta_f$, $\Delta\eta_s$, β_s^0 , and β_f^0 .

Firstly, the parameter $\Delta\beta_s$ is tested with four values, $\Delta\beta_s = 0.5$, $\Delta\beta_s = 0.75$, $\Delta\beta_s = 1.0$, and $\Delta\beta_s = 2.0$, with two other parameters set as $\Delta\beta_f = 0.5$ and $\Delta\eta_s = 0.01$, respectively. The corresponding optimization results are shown in Fig. 4.9, which share similar structural topologies. The static compliance values of optimized coated cantilever beams are given in Table 4.2. Taking the design considering $\Delta\beta_s = 0.5$ as a reference, differences between their final structural performance are also presented. Among them, the largest value of the parameter $\Delta\beta_s$ generates the worst structure, whose compliance value is 6893.58 and has a 2.06% growth compared to the reference one. This phenomenon is because the substrate region of a coated structure is premature with a large $\Delta\beta_s$ value and the design freedom is thus limited. With the other three values of $\Delta\beta_s$,

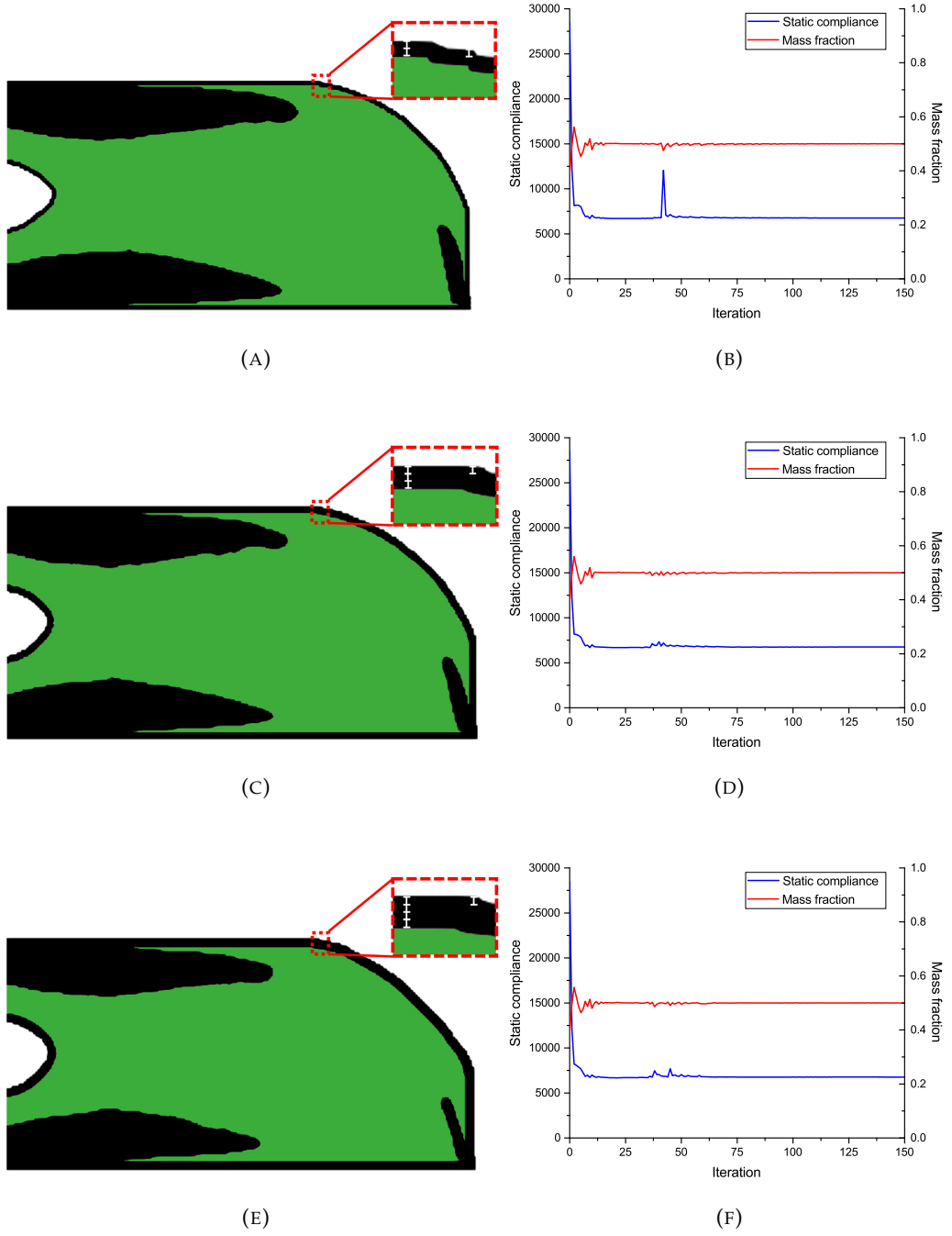


FIGURE 4.8: Optimized results of the cantilever beam with different coating thicknesses: (a) and (b) using $w_e = 2$; (c) and (d) using $w_e = 3$; (e) and (f) using $w_e = 4$.

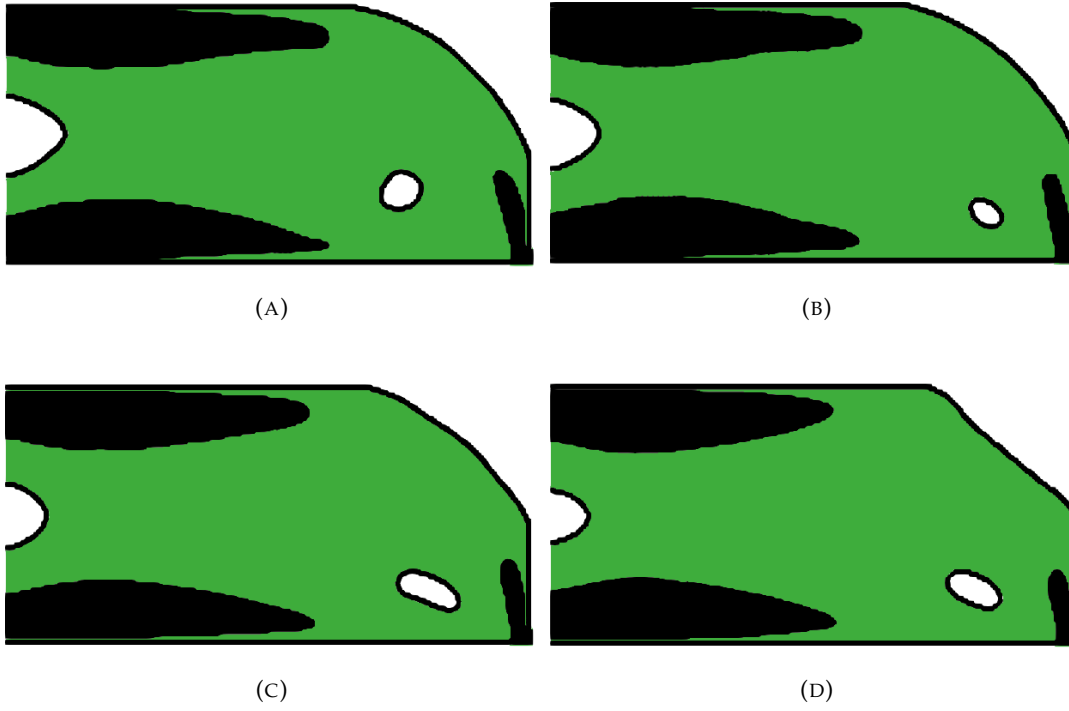


FIGURE 4.9: Optimized results of the cantilever beam with different $\Delta\beta_s$: (a) $\Delta\beta_s = 0.5$; (b) $\Delta\beta_s = 0.75$; (c) $\Delta\beta_s = 1.0$; (d) $\Delta\beta_s = 2.0$.

optimized coated structures have almost the same compliance value. To conclude, the increment of the sharpness parameter $\Delta\beta_s$ has limited effect on optimized structural topology but certain influence on final structural performance. Numerical tests reveal that the value of $\Delta\beta_s$ is expected to be smaller or equal to 1.0.

It is interesting that the topologies presented in Fig. 4.9 all have a void hole in their lower right parts but those as shown in Fig. 4.8 do not have this structural characteristic. In our opinion, such a difference in the structural topology is mainly caused by the different $\Delta\beta_f$ we set for them. To be specific, $\Delta\beta_f$ is defined as 0.5 and 1.0 for those presented in Fig. 4.9 and Fig. 4.8, respectively. The term $\Delta\beta_f$ determines the growth of β_f for the Heaviside projections (with the $\Delta\beta_f = \Delta\beta_e$ setting) and a larger $\Delta\beta_f$ will offer a strong projection effect earlier during the iteration. In this way, an area of large density values during the early optimization process will be directly projected as an infilling material and cannot nucleate holes anymore, as shown in Fig. 4.8, due to the large value of β_f reaches. On the contrary, with a smaller $\Delta\beta_f$ value, the projections applied to this area are not strong and it can be further optimized as an internal hole, as presented in Fig. 4.9.

Next, we consider the parameter $\Delta\beta_f$ with four different values, $\Delta\beta_f = 0.5$, $\Delta\beta_f = 0.75$, $\Delta\beta_f = 1.0$, and $\Delta\beta_f = 2.0$. The other two parameters are set as $\Delta\beta_s = 0.5$ and $\Delta\eta_s = 0.01$. Since the case of $\Delta\beta_f = 0.5$ and $\Delta\beta_f = 1.0$ have already been respectively shown in Fig. 4.9a and Fig. 4.8a, they are not presented in this subsection to avoid the repetition of figures and other corresponding

TABLE 4.2: Properties of the optimized cantilever beam with different $\Delta\beta_s$.

$\Delta\beta_s$	$\Delta\beta_f$	$\Delta\eta_s$	Objective	Difference (%)
0.5	0.5	0.01	6754.23	0.00
0.75	0.5	0.01	6751.91	-0.03
1.0	0.5	0.01	6787.80	0.50
2.0	0.5	0.01	6893.58	2.06

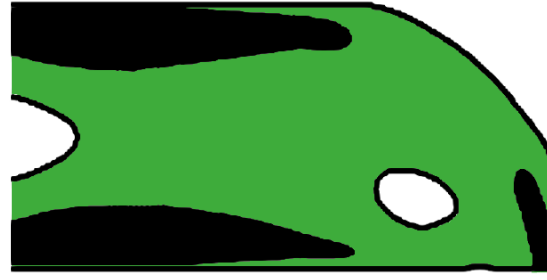
FIGURE 4.10: Optimized results of the cantilever beam with different $\Delta\beta_f$: (a) $\Delta\beta_f = 0.75$; (b) $\Delta\beta_f = 2.0$.

optimization results are shown in Fig. 4.10. The layout patterns of materials are almost the same, with the material 2 mainly concentrated near the fixed and the loading boundaries. However, it can be observed that with a larger parameter $\Delta\beta_f$ than $\Delta\beta_s$, the optimized structures have no holes generated within the design domain. The structural performance and the numerical difference are summarized in Table 4.3. According to the numerical values, it can be seen that differences of structural performance are all within -0.5% , thus, the parameter $\Delta\beta_f$ may have little influence on the optimized topology and structural performance using the proposed approach.

Finally, the increment of the threshold parameter $\Delta\eta_s$ is studied. Similarly, four different values are allocated for the $\Delta\eta_s$ as $\Delta\eta_s = 0.005$, $\Delta\eta_s = 0.01$, $\Delta\eta_s = 0.02$, and $\Delta\eta_s = 0.03$. Other two considered parameters are set as $\Delta\beta_s = 0.5$ and $\Delta\beta_f = 0.5$, respectively. The case of $\Delta\eta_s = 0.01$ is the same as the case of $\Delta\beta_f = 0.5$ discussed before, with optimized design shown in Fig. 4.9a. Fig. 4.11 presents the optimization results of the three other cases. Different from $\Delta\beta_s$ and $\Delta\beta_f$,

TABLE 4.3: Properties of the optimized cantilever beam with different $\Delta\beta_f$.

$\Delta\beta_s$	$\Delta\beta_f$	$\Delta\eta_s$	Objective	Difference (%)
0.5	0.5	0.01	6754.23	0.00
0.5	0.75	0.01	6740.98	-0.20
0.5	1.0	0.01	6737.52	-0.25
0.5	2.0	0.01	6727.09	-0.40



(A)



(B)



(C)

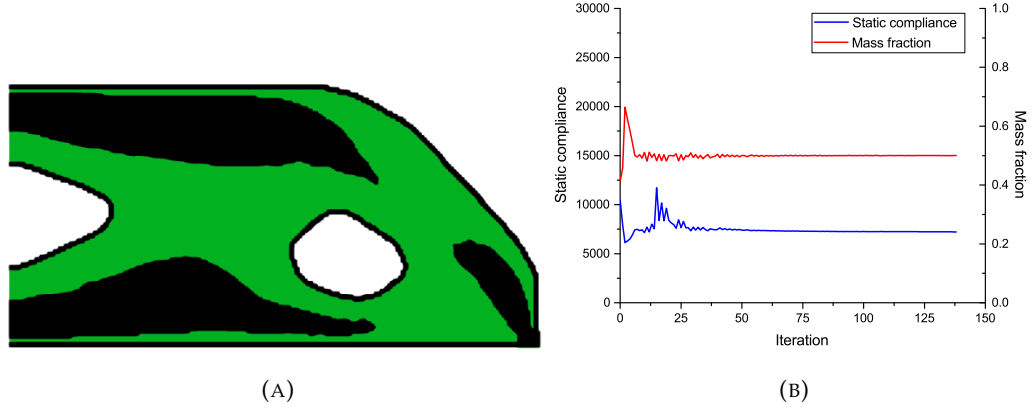
FIGURE 4.11: Optimized results of the cantilever beam with different $\Delta\eta_s$: (a) $\Delta\eta_s = 0.005$; (b) $\Delta\eta_s = 0.02$; (c) $\Delta\eta_s = 0.03$.

varied values of the parameter $\Delta\eta_s$ generate different structural topologies, especially greatly affect the layout of the material 2 within the substrate of coated structures. When $\Delta\eta_s = 0.02$ and $\Delta\eta_s = 0.03$, there are many isolated distributions of the material 2 within the optimized coated structures as shown in Fig. 4.11b and Fig. 4.11c, which cannot effectively resist the external loads. However, numerical differences of them are smaller than 2.0%, which proves the effectiveness of the proposed method. These numerical tests reveal that the parameter $\Delta\eta_s$ has certain effects on the topology of optimized structures since a large value of $\Delta\eta_s$ leads to an earlier identification of the coating and the substrate, restricting the design freedom during the optimization. Numerically, we suggest the value of $\Delta\eta_s$ be smaller than 0.01 for a better structural performance.

Next, the influence of β_s^0 on optimization result is investigated. Based on the setting of the

TABLE 4.4: Properties of the optimized cantilever beam with different $\Delta\eta_s$.

$\Delta\beta_s$	$\Delta\beta_f$	$\Delta\eta_s$	Objective	Difference (%)
0.5	0.5	0.005	6823.72	0.00
0.5	0.5	0.01	6754.23	-1.02
0.5	0.5	0.02	6918.70	1.39
0.5	0.5	0.03	6937.06	1.66

FIGURE 4.12: Optimization results of the cantilever beam using $\beta_f^0 = 8$: (a) optimized structure; (b) iteration history.

numerical example presented in Section 4.5.1 with the coating thickness as $w_e = 2$, the value of β_s is re-initialized as $\beta_s^0 = 8$. The optimized structural configuration of the cantilever beam and its iteration history are presented in Fig. 4.12a and Fig. 4.12b, respectively. As can be observed, the topology obtained using $\beta_s^0 = 8$ is different from the one using $\beta_s^0 = 1$ (as shown in Fig. 4.8a) with a huge void in its right part. The generation of this hole can be mainly attributed to the premature of the infilling area caused by a large value of β_s , with the influence of other design parameters. According to the iteration history presented in Fig. 4.12b, a large β_s^0 value leads to several ups and downs during the early optimization process. On the contrary, the setting of $\beta_s^0 = 1$ leads to a more stable iteration process as presented in Fig. 4.8b, which shows the initial value of β_s has certain effect on the iteration performance. The final static compliance value is $c = 7223.67$. Even though the optimization terminates earlier with a lower computational time (334s) and a smaller total iteration steps (138 steps), the result using $\beta_s^0 = 8$ has a 7.2% larger compliance value compared to the structure using $\beta_s^0 = 1$ as shown in Fig. 4.8a, proving the advantage of using a small β_s^0 value in the proposed method. Through this example, it can be concluded that a small β_s^0 value is better for obtaining results with great structural performance and generating stable iteration performance using the proposed method.

As the final design parameter to be studied, the term β_f^0 is given as $\beta_f^0 = 2$ to test its effect on optimization results. Other design parameters are kept the same as those for the result presented in Fig. 4.8a. Fig. 4.13 shows the optimized cantilever beam and its iteration history. Generally, the

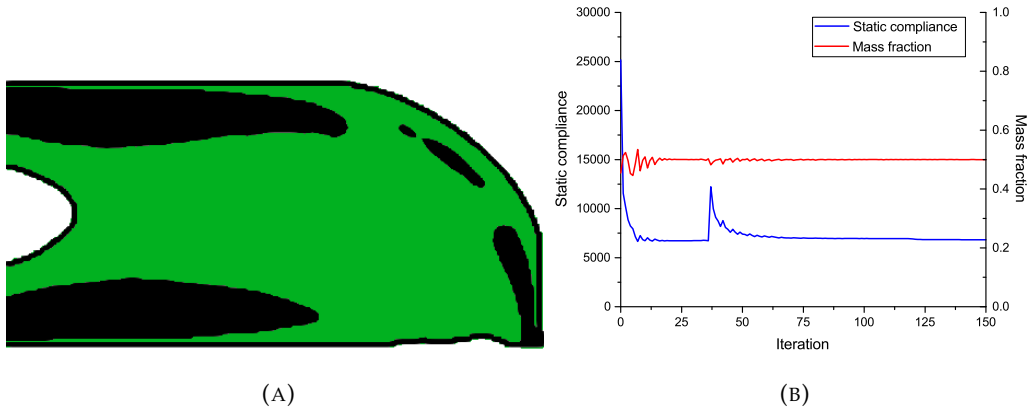


FIGURE 4.13: Optimization results of the cantilever beam using $\beta_f^0 = 2$: (a) optimized structure; (b) iteration history.

structural topologies as shown in Fig. 4.8a and Fig. 4.13a have certain similarities. However, we can observe that some isolated areas of the material 2 exist within the optimized coated structure using $\beta_f^0 = 2$. The reason for this phenomenon is mainly due to the comparatively large β_f which projects the density within the coated structure to the material 2 in an early way. The final static compliance value is obtained as $c = 6827.65$, which is 1.3% larger than that of the structure using $\beta_f^0 = 1$. The total computation time is 364s, similar to the 352s consumed by the result as shown in Fig. 4.8a. Regarding to the iteration performance, the general trend of the iteration between Fig. 4.8b and Fig. 4.13b is the same. However, it can be clearly seen that many small obvious fluctuations exist on the curve of the objective function. Therefore, the optimization using $\beta_f^0 = 1$ has the better iteration performance with lower static compliance value.

4.5.2 MBB beam

Here, a modified MBB (Messerschmitt Bolkow Blohm) beam structure is considered for further numerical tests. The geometrical dimensions and boundary conditions of it are presented in Fig. 4.14. Two materials are also considered in this example, with their defined properties given in Table 4.4 and the coating is made of the material 2. The effect of different material properties and varied mass constraints on optimized designs are studied. Other design parameters are set as $\Delta\beta_M = 0.25$, $\Delta\eta_s = 0.01$, and $\Delta\beta_f = 0.5$. The maximum allowed mass fraction is set as $M_f = 45\%$. Thickness of the coating is set as $w_e = 2$, leading to the radius parameter $R_e = 3$. The minimum and the maximum iteration numbers for the iteration are also given as $I_{\min} = 100$ and $I_{\max} = 150$, respectively.

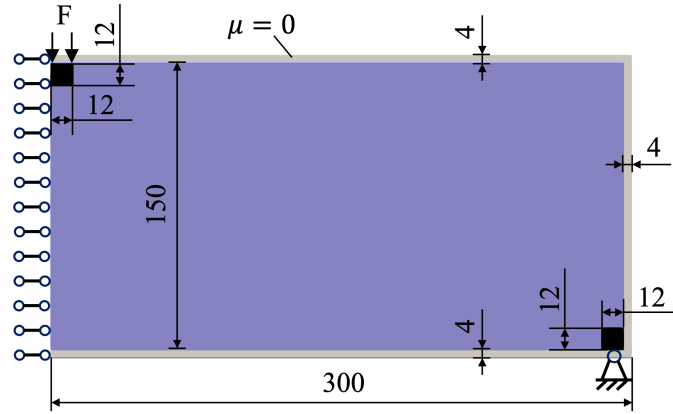


FIGURE 4.14: Design domain of the modified MBB beam.

TABLE 4.5: Properties of the considered materials for the MBB beam.

Name	Normalized density	Young's modulus	Mass	Color
Void	0	0	0	White
1	0.5	(not defined)	(not defined)	Green
2	1.0	1.0	1.0	Black

Different material properties

Three groups of material properties are specified for the material 1, i.e., (a) $E_1 = 0.5$, $M_1 = 0.3$; (b) $E_1 = 0.5$, $M_1 = 0.4$; (c) $E_1 = 0.5$, $M_1 = 0.5$, are used to test how can the material properties affect final optimized structures. The corresponding optimization results are presented in Fig. 4.15. Generally, the optimized MBB beams all have arch-bridge like shapes and their external coatings greatly cover the infill materials. Among all optimized structures, the material 2 works as the main material for the load transfer due to its larger Young's modulus, which greatly link the loading position to the fixed boundaries within the substrate region. Besides, it can be observed that the thickness of the coating is well-maintained in all the cases and all the infilling materials are greatly covered by the external coating. With the increment of the mass of the material 1 from Case (a) to Case (c), more holes are generated and much more mass resource is assigned to the material 2, as presented in Fig. 4.15. Such a tendency is reasonable, because the material 1 is less preferable in the coated structure when its mass increases, due to its lower stiffness-to-weight ratio compared to the material 2. In other words, when the same mass resource is allocated, the structure prefers to use less material 1 but much more material 2 for better structural performance. The static compliance value of the optimized structures grows in a monotonic trend when the mass of the material 1 keeps growing, which are (a) $c = 2955.15$, (b) $c = 3038.01$, and (c) $c = 3129.76$, respectively. Thus, from this numerical test, we can find that the material properties of the infill materials have an important influence both on the optimized material distribution and the final objective value. Specially, at the lower part of the structure presented in Fig. 4.15a, the infilling material 2 is connected to the outer coating by the infilling material 1. In our opinion, the reason

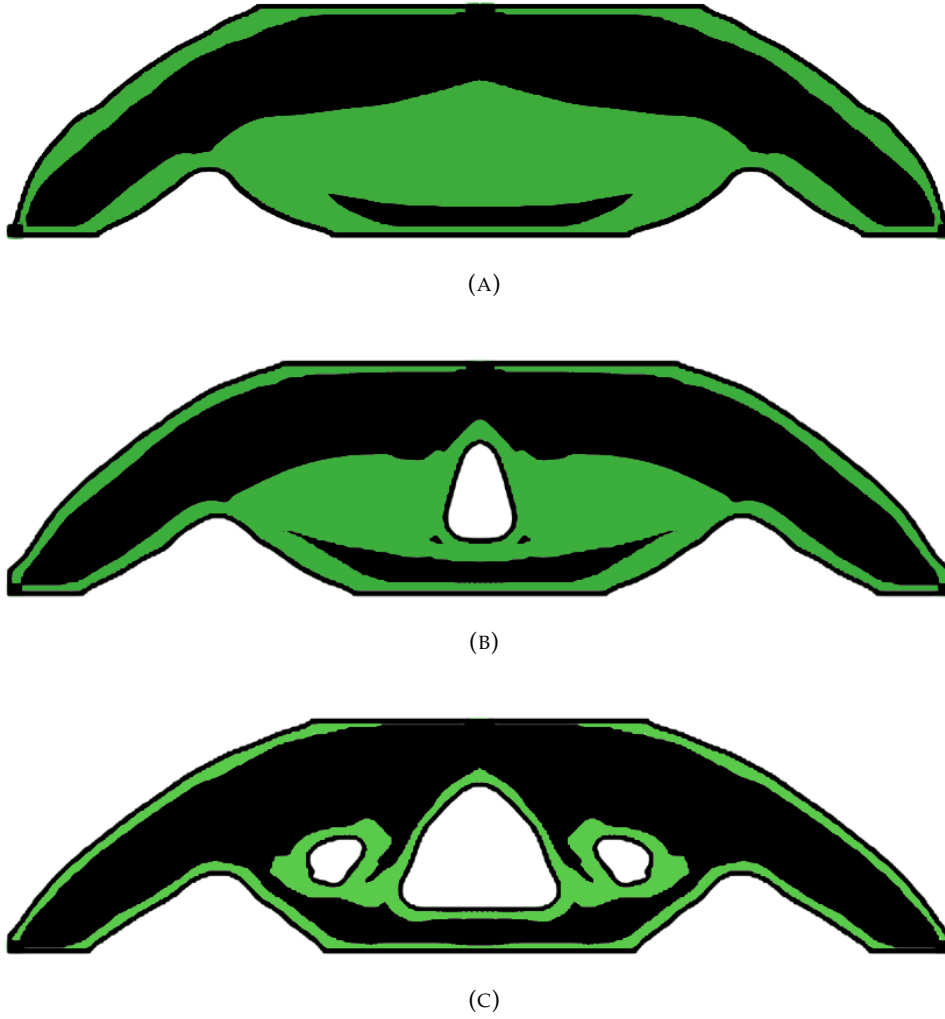


FIGURE 4.15: Optimized results of the MBB beam with varied properties of the material 1: (a) $E_1 = 0.5$, $M_1 = 0.3$; (b) $E_1 = 0.5$, $M_1 = 0.4$; (c) $E_1 = 0.5$, $M_1 = 0.5$.

of this phenomenon might be the higher stiffness-to-weight ratio of the material 1 and the strong Heaviside projection effects during the optimization.

Different mass constraints

This subsection tests the effectiveness of the considered mass constraint and three different maximum mass fractions are introduced, i.e., $M_f = 30\%$, $M_f = 50\%$, and $M_f = 70\%$. The material properties of the material 1 are set as $E_1 = 0.5$ and $M_1 = 0.4$. Fig. 4.16 presents the corresponding optimization results. As can be seen, different mass constraints can generate varied structural topologies. In general, the optimized MBB beams still have the arch-bridge like topologies, transferring the external loads to the fixed boundaries at both ends of the beam. However, similar distribution of the material 2 within the substrate can be observed among these three designs,

which effectively transfer the loads and resist the deformation of the MBB beam with its larger stiffness-to-weight ratio. When the allowed maximum mass fractions grows up, the percentage of the material 2 consumption within the substrate also increases, revealing the algorithm still prefers the material 2 to better resist the structural deformation. The MBB beam structures optimized using the proposed method shown in Fig. 4.16 all have an external coating with uniform thickness. Besides, with a larger allowed maximum mass fraction, the final structural performance is improved and the static compliance values of the designs we obtained are $c = 4677.03$, $c = 2968.50$, and $c = 2500.12$, respectively. A coating collision can be observed on Fig. 4.16b, in which coatings are merged at the central area of the structure. From the AM perspective, this structural characteristic is manufacturable and it can contribute a better structural performance, even though it can be avoided via a minimum length scale restriction. However, to ensure the manufacturability of optimized results, many possible solutions can be introduced to control the minimum-length scale, such as the geometric constraint (Zhou, Lazarov, Wang, and Sigmund, 2015) and the worst-case robust formulation (Sigmund, 2009). Recently, a novel and pioneering explicit minimum length-scale restriction has been proposed by Postigo et al. (Postigo, Garaigordobil, Ansola, and Canales, 2024) to control the minimum length-scale based on the skeleton recognition of the structure.

In the presented examples, two infilling materials are considered for MBB beams and the material 2 (with higher stiffness) has constructed the main routine for the load transfer. In our opinion, different design freedom is the main reason for obtaining different structural topologies when considering the single-material MBB beam and the coated MBB beam with two infilling materials. Besides, design parameters for multiple filtering and projections can also greatly affect the optimization results. Upon closer observation, it can be noted that the distribution of the shell and the material 1 primarily revolves around the material 2, serving as supplementary means to enhance structural stiffness and transmit loads.

4.5.3 Simply supported bridge

Considering the pressure load, Fig. 4.17 shows the geometrical dimension and the boundary condition of a 2D bridge. In this example, optimization of coated structures considering three materials is investigated, whose properties are listed in Table 4.6. The material 3 is selected for the coating construction and the thickness of the coating is defined as $w_e = 2$. The mass constraint is given as $M_f = 50\%$. Other corresponding design parameters are set as $\Delta\beta_M = 0.25$, $\Delta\eta_s = 0.01$, and $\Delta\beta_f = 0.5$, respectively.

Different number of infill materials

To test the advantages of considering multi-material infilling in the design of coated structures, we conduct topology optimization of the 2D bridge with different infill materials, including infilled

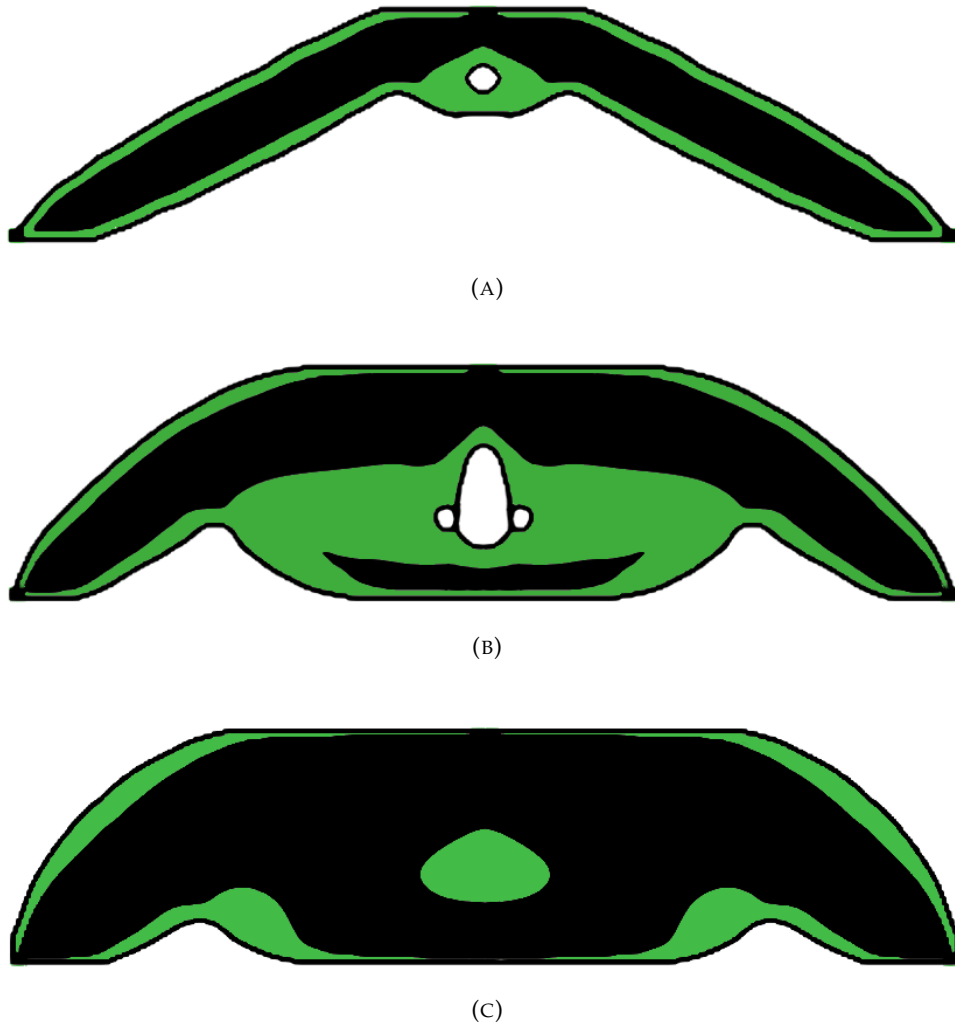


FIGURE 4.16: Optimized results of the MBB beam infilled with two materials considering different mass constraints: (a) $M_f = 30\%$; (b) $M_f = 50\%$; (c) $M_f = 70\%$.

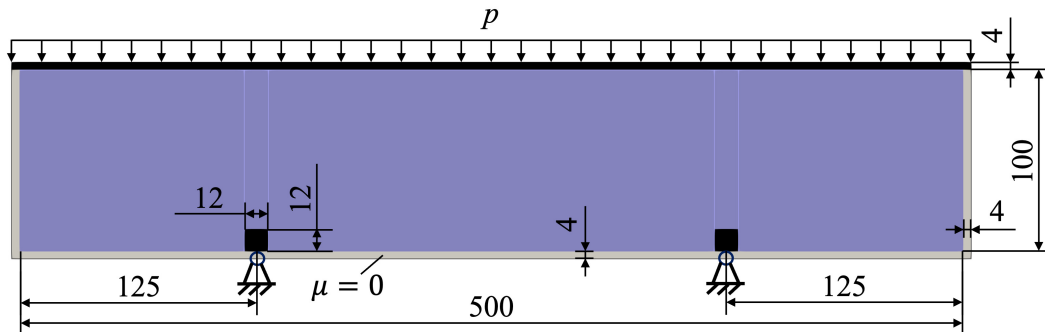


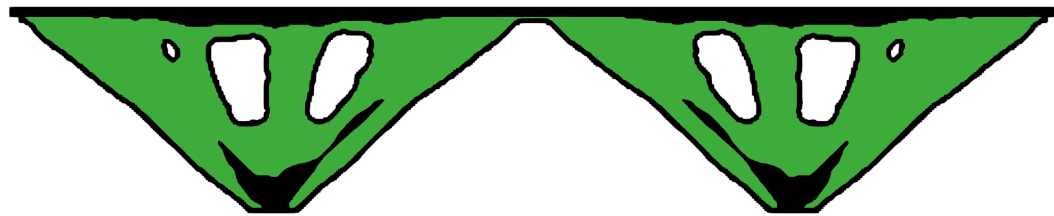
FIGURE 4.17: Design domain of the 2D bridge.

TABLE 4.6: Properties of the considered materials for the 2D bridge.

Name	Normalized density	Young's modulus	Mass	Color
Void	0	0	0	White
1	0.4	0.2	0.5	Green
2	0.7	0.6	0.8	Orange
3	1.0	1.0	1.0	Black



(A)



(B)



(C)

FIGURE 4.18: Optimized results of the 2D bridge infilled with (a) the material 1; (b) the material 1 and the material 2; (c) the material 1, the material 2, and the material 3.

with only the material 1 (traditional shell-infill structures), with the material 1 and the material 3, and with all of three materials. The corresponding optimization results are presented in Fig. 4.18 and the single infilling material case is optimized using the erosion-based TO method proposed by Luo et al. (Luo, Li, and Liu, 2019). Obviously, coated bridges we obtained have different structural topologies. Compared to the structure shown in Fig. 4.18a, considering multiple infill materials lead to the nucleation of holes within the substrate region. With the largest Young's modulus and density values, the material 3 mainly concentrated near the fixed boundaries and a small amount of the material 3 is generated beneath the top loading boundary in the cases of multiple infill materials. In addition, the consideration of multiple infill materials in both of two examples lead to a better structural performance than the single infill material case ($c = 506456$) as shown in Fig. 4.18a, revealing the potential of designing coated structures infilled with multiple materials. Moreover, it is interesting that the introduction of the material 2 for the infilling generates the design shown in Fig. 4.18c with a lower static compliance value ($c = 412456$) than the one presented in Fig. 4.18b ($c = 487103$). This means that the increment of infill materials has the ability to enable coated structures with a better structural performance under the same structural mass. Through this example, the advantages of coated structures infilled with multi-phase materials and the effectiveness of the proposed topology optimization method are well illustrated.

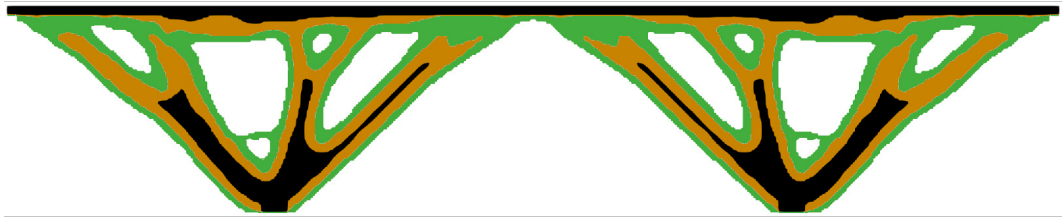
Considering no outer coating

To better illustrate the advantage of designing coated structures, a 2D three-material bridge without the outer coating is considered in this subsection. Materials listed in Table 4.6 are used to construct the structure and other corresponding design parameters are the same as those used for the result as shown in Fig. 4.18c. Fig. 4.19 presents the optimized structural configuration of the 2D three-material bridge. As can be seen, the bridge is mainly composed of the material 1 and the distribution of the material 3 mainly concentrates near the fixed boundaries, as those presented in Figs. 4.18b and c. Under the same mass constraint and compared to its coated one, the 2D three-material bridge without the coating as shown in Fig. 4.19 has more branches made of the material 2 to resist the deformation caused by the external load. However, its final static compliance value is $c = 460846$, which is more than 10% higher than that of its coated one. Through this example, it can be concluded that the consideration of the outer coating can lead to a better structural performance in the multi-material design under the mass consumption constraint, proving the advantage of designing coated structures.

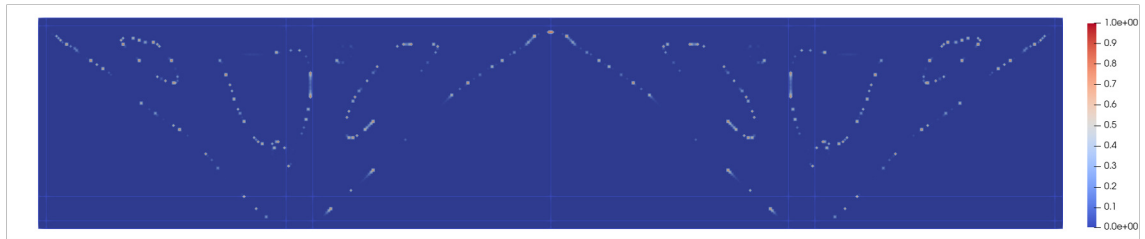
To investigate the possibility of designing multi-material structures with no coating using the proposed method, we directly set the term ω_e as $\omega_e = 0$ based on the three-material bridge example with other design parameters remain. Under the same mass constraint, the optimization result is presented in Fig. 4.20. Although the main distributions of considered materials are similar in both cases, there are certain differences between the one obtained by the ordered SIMP



FIGURE 4.19: Optimized 2D three-material bridge without the outer coating using the ordered SIMP method.



(A)



(B)

FIGURE 4.20: Optimized 2D three-material bridge without the outer coating using the proposed method with the setting $\omega_e = 0$.

method (Fig. 4.19) and the result as shown in Fig. 4.20a. As the main difference, there is less material 1 and much more material 3 generated in the case of $\omega_e = 0$. The static compliance value of the obtained result is $c = 463135$, which is about 0.5 % larger than the one using the ordered SIMP approach. However, we can find that limited amount of the "coating" being identified, as presented in Fig. 4.20b. Therefore, in our opinion, the developed approach for coated structures infilled with multiple materials has certain ability to design structures with no coating, but the introduced strict Heaviside projection and the two-step filtering are not necessary in this case and both of them have certain effect on the optimization result.

3D bridge

The final example is a design problem of a 3D simply supported bridge considering the pressure loads applied on its top surface, which is illustrated in Fig. 4.21. For a better illustration, the design and the non-design domains are depicted in light blue and purple, respectively. With the

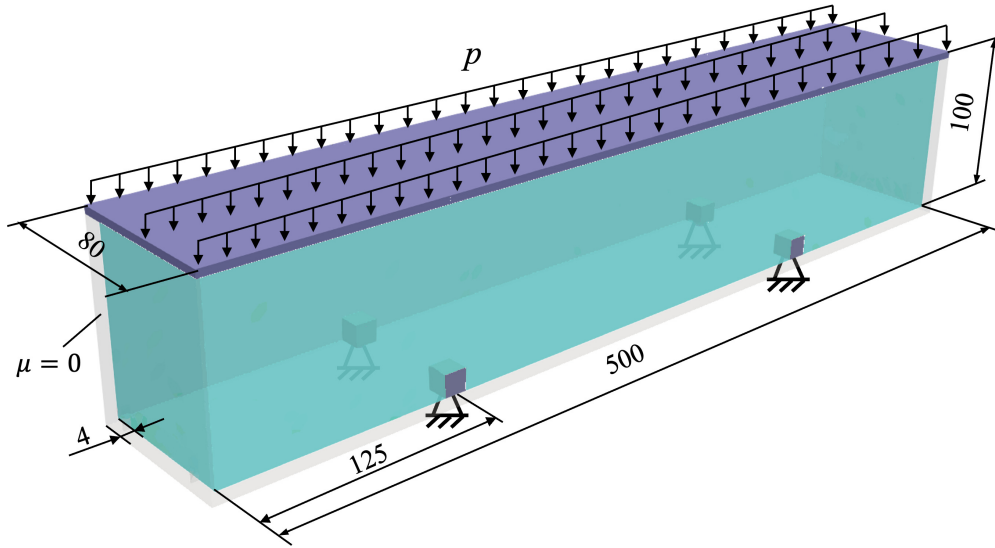
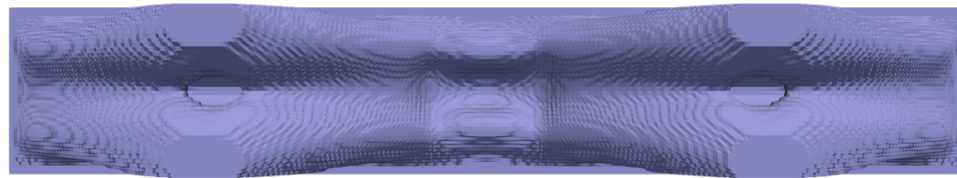


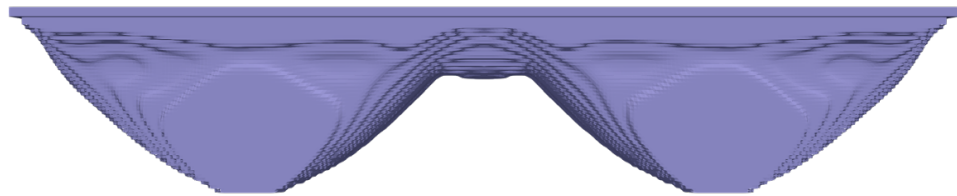
FIGURE 4.21: Design domain of the 3D bridge.

same material properties as the 2D case, the three-material infilling is considered in this example and the material of the coating is assumed as the material 3 due to its largest Young's modulus value. The mass constraint is defined as $M_f = 35\%$. Using the parallel computation, the overall optimization result is shown in Fig. 4.22 with different view directions. Basically, the material distribution of the optimized 3D coated bridge has some similarity with the 2D cases, but no connected holes are nucleated on the 3D optimized result. On the contrary, there are two big void domains formed by the topology of the external coating, which can be observed from the bottom view given in Fig. 4.22a. To effectively resist the structural deformation, the coating we optimized under the defined conditions has continuous material distribution from the top loaded surface to the bottom fixed surfaces, which effectively cover all the infill materials.

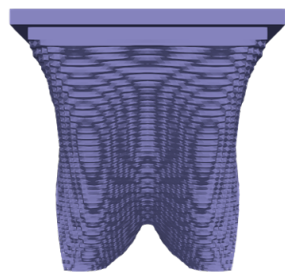
In order to clearly present the optimized material layout, one fourth of the whole 3D bridge is considered and the distribution of the material 1, the material 2, and the material 3 are shown in Fig. 4.23a, Fig. 4.23b, and Fig. 4.23c, respectively. As the main infill material, the material 1 occupies most of the substrate domain. Apart from some distributed beneath the top loaded surface, we can see that the layout of the material 2 mainly concentrate near the supporting surfaces from Fig. 4.23b, which has two branches to better withstand and transfer the pressure loads from the top to the bottom supported areas. Varied from the material 1 and the material 2, a few material 3 is obtained as the infill for the three-material infilling and all focus near the supporting boundaries. Such a phenomenon can be attributed to the large mass resource consumption by the external coating. The topology of the optimized external coating is given in Fig. 4.23d in details. As can be seen, the huge void domain mentioned before is formed by the coating. Therefore, the external pressure loads can be transmitted to the supporting areas in a higher efficiency. Besides, the uniform thickness of the external coating is well controlled, proving the effectiveness of the proposed scheme. Fig. 4.23e and Fig. 4.23f are two section views of the one fourth of the optimized bridge, which offer more information about the material layout within the substrate.



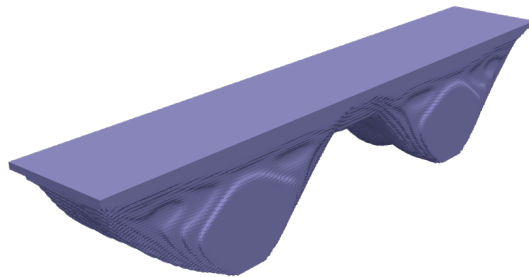
(A)



(B)



(C)



(D)

FIGURE 4.22: The optimized topology of the 3D bridge: (a) the bottom view; (b) the front view; (c) the left view; and (d) the isometric view.

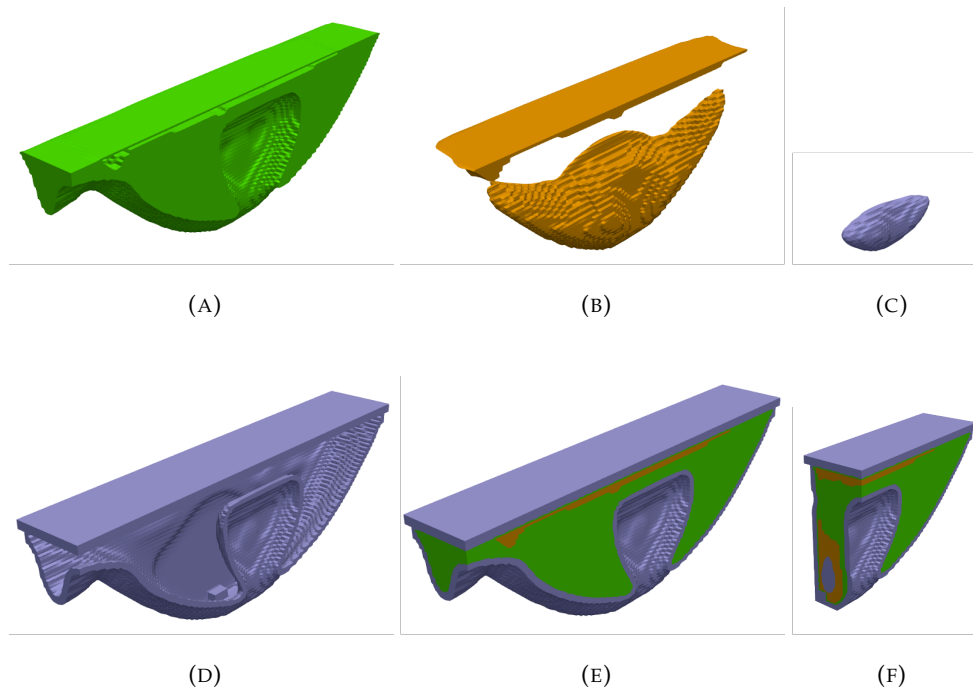


FIGURE 4.23: Material layout of (a) the material 1; (b) the material 2; (c) the material 3; (d) the external coating; and section views (e) and (f) of the one fourth of the optimized 3D bridge.

With clear material distribution of the external coating and the multi-material infilling, the structural deformation induced by the external pressure loads can be greatly resisted. Through this example, the effectiveness of the proposed method for 3D optimization problems is also illustrated. However, the 3D optimization results we obtained do have obvious zig-zag structural boundaries, mainly due to the density method and the comparatively large element size we implemented. To deal with this issue, many special techniques can be further introduced, such as the body-fitted mesh (Feppon, Allaire, Dapogny, and Jolivet, 2020).

4.6 Summary

This paper proposes an ordered SIMP-based method to deal with topology optimization of coated structures with multiple infill materials. A new filtering and projection procedure is developed to identify the external coating and describe the layout of multiple infill materials, where the frequently-used PDE filtering and tanh-function-based Heaviside projection are utilized. Using multiple modified density fields and no gradient calculation, the construction of coated structures and thickness control of the external coating have been presented. Then, a new ordered SIMP-based material interpolation scheme is developed to describe the material properties of coated

structures. With a total mass constraint, the mathematical model for the minimization of structural static compliance is constructed and sensitivities are derived in detail. The validity and effectiveness of the proposed method are demonstrated by several 2D and 3D numerical examples. Results illustrate that the multi-material infilling within coated structures can be described and optimized effectively. Besides, the thickness of the external coating can be well handled by an eroded density field and its original field under the effect of corresponding design parameters.

With the development of additive manufacturing (AM) technique, the method proposed in this paper offers a possibility to consider multi-material infilling for the design of coated structures using the density-based method. According to the numerical tests on design parameters, the authors admit that the proposed method has certain parameter dependence on obtaining reasonable and effective structural topologies. However, the results optimized using the developed approach still have acceptable structural performance due to the multi-material infilling we considered, along with great simplicity to implement and stable iteration history. The proposed multi-material TO method for the design of coated structures can be used for various engineering application, such as designing multi-material bus frames (Lu, Ma, Xin, and Zuo, 2019). In addition, the developed method can be further extended to achieve the design of coated structures infilled with multiple lattice microstructural materials for lightweight design (such as the lattice structured pillow bracket (Zhang, Liu, and To, 2017)) and achieve special functionalities (such as the bone implant (Zhang, Takezawa, Ding, Xu, Duan, Li, and Guo, 2021)), which will be discussed by us in the near future.

Chapter 5

Multiscale topology optimization of coated structures with multiple self-connected microstructures [†]

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[†]The work in this chapter has been submitted for review in *International Journal for Numerical Methods in Engineering* (Wiley), 2024.

5.1 Introduction

Widely regarded as a powerful structural design technique, topology optimization (TO) owns a distinct ability in determining the optimal material distribution to achieve expected structural performance while satisfying a set of constraints without prior knowledge. Since the pioneering work of Bendsøe and Kikuchi (Bendsøe and Kikuchi, 1988), this novel technique has undergone vigorous development, especially with an easier fabrication of optimized structures using the AM technique. Many effective TO methods have been proposed in the TO community, including the level set (LS)-based method (Xia, Shi, and Wang, 2011; Wang, Kang, and Liu, 2019), the SIMP method (Bendsøe and Sigmund, 1999), the evolutionary structural optimization (ESO)/bi-directional ESO (BESO) method (Xie and Steven, 1993; Huang, Xie, and Burry, 2006), the moving morphable components/voids (MMC/MMV) method (Guo, Zhang, and Zhong, 2014; Zhang, Chen, Zhu, Zhou, Xue, Lei, and Guo, 2017), etc. Over decades of development, TO has been successfully employed on various engineering problems, including stiffener layout optimization (Lei, Xiaohong, Tiannan, Xiong, and Zhang, 2022; Hu, Ding, Shen, and Zhang, 2020), thermal-fluid system design (Wang, Wang, Liu, Dbouk, Peng, and Ali, 2023; Yaji, Yamada, Kubo, Izui, and Nishiwaki, 2015), vibration mitigation (Matlack, Bauhofer, Krödel, Palermo, and Daraio, 2016; Zhao, Feng, Li, and Xue, 2022), meta-material design (Li, Gao, Wang, and Luo, 2022; Gao, Cao, Xiao, Yang, Zhou, Li, Gao, Yan, Rabczuk, and Mai, 2023; Li, Gao, Kessissoglou, Oberst, Wang, and Luo, 2023), etc.

Getting inspiration from the natural realm, coated structures infilled with lattice microstructures are composed of a solid external coating and internal lattice material. Functionally, the outer coating can offer protection to the substrate of coated structures and further improves certain structural performance (e.g. buckling resistance ability (Clausen, Aage, and Sigmund, 2016)). Usually made of uniform and periodic arrangement of porous microstructures, lattice material exhibits attractive mechanical properties, such as high stiffness/strength-to-weight ratio and excellent energy absorption capability, making it suitable for the substrate of coated structures. In addition, microstructures can offer physical support to the outer coating during the AM process. Attracting increasing attention from academia to industry, coated structures with lattice microstructural infilling have presented its great potential in varied applications (Heimann and Lehmann, 2015; Niu and Wadbro, 2021).

Stimulated by Clausen et al. (Clausen, Aage, and Sigmund, 2015), designing coated structures infilled with porous microstructures has become a popular topic in the field of TO and many research achievements have been conducted. For example, Liu et al. (Liu, Zhou, Wei, and Lin, 2021) proposed a density-based method to generate self-supporting infill structures for given prototypes. Wu et al. (Wu, Aage, Westermann, and Sigmund, 2017) optimized bone-like porous structures for coated structures by introducing local volume constraints. Different from these single-scale TO works focus on the infilling, multiscale TO owns a much larger design freedom and can lead to a better structural performance by considering the interaction of structural evolution at two scales. However, how to effectively distinguish the coating, the substrate, and the

void domain at the macroscale level is critical in multiscale TO of coated structures. To deal with this issue, LS methods show great advantages due to their implicit structural representation using level set surfaces and different domains can be determined according to varied LS values. Especially, the coating thickness can be well described by using two LSs of a single LS function thanks to the signed distance property. Wang and Kang (Wang and Kang, 2018a) firstly designed 2D and 3D coated structures based on the LS method. Fu et al. (Fu, Li, Gao, and Xiao, 2019) proposed a multiscale parametric LS-based TO method for the design of coated structures with periodic lattice microstructures. Based on the velocity field-based LS method, Hu et al. (Hu, Wang, Zhang, Li, Ding, Izui, and Nishiwaki, 2022; Hu, Wang, Zhang, Li, Ishida, Sasaki, Furuta, Izui, and Nishiwaki, 2023) developed multiscale TO of coated structures infilled with microstructures considering dynamic structural performance. As for the density-based method, smoothing and projection operations are often introduced for the coating identification. In the research of Clausen et al. (Clausen, Aage, and Sigmund, 2015), the coating is identified by a two-step filtering and the spatial gradient of the density field. Chu et al. (Chu, Xiao, Gao, Li, Zhang, and Zhang, 2019) further developed an extended two-step filtering scheme to identify the interfaces between different materials of multi-material structures, in which two sets of design variables are respectively smoothed and projected to search the optimal multi-material distribution. Without gradient calculation, Yoon and Yi (Yoon and Yi, 2019) constructed a simple density-based procedure for the modelling of the outer coating by multiplying the modified density fields with the original design variables. Subsequently, Yi et al. (Yi, Yoon, and Peng, 2021) updated the procedure in (Yoon and Yi, 2019) and found the coating with two-step filtered densities during the optimization. In the research work of Zhou et al (Zhou, Lu, Liu, and Lin, 2022), two density variable fields are introduced to distinguish the void, the coating, and the infills, using the combination of modified variables. Luo et al. (Luo, Li, and Liu, 2019) presented an erosion-based identification method to design coated structures and the theoretical derivation for the control of coating thickness was also conducted. Even though the coating and the infilling regions can be clearly distinguished, it should be noted that the above-mentioned density-based approaches can only deal with the single infilling material/microstructure.

Recently, one of the popular trends towards multiscale coated structure design is to consider inhomogeneous microstructures as the lattice infilling, which can exhibit better structural performance than those infilled with the periodic pattern of a single microstructural configuration. To achieve such inhomogeneous material properties, various strategies have been developed. Wei et al. (Wei, Ye, Zhang, Li, and Sui, 2022) considered multiple predefined microstructures and optimized the distribution of them on the macrostructure. Zhou et al. (Zhou, Lu, Liu, and Lin, 2022) concurrently optimized geometries of the coating and the inhomogeneous infilling with consideration of the overhang constraint. An easy way to achieve inhomogeneous material properties is generating lattice infilling formed by various layers of different periodic microstructures. Following the strategy proposed by Zhang et al. (Zhang, Wang, and Kang, 2019), the substrate of coated structures is uniformly divided into different layers and layer-wise microstructural infilling is optimized in the research of (Hu, Wang, Zhang, Li, Ding, Izui, and Nishiwaki, 2022; Hu, Wang,

Zhang, Li, Ishida, Sasaki, Furuta, Izui, and Nishiwaki, 2023). Li et al. (Li, Luo, Gao, and Walker, 2018) also designed functionally graded cellular composites hosting auxetic metamaterials by dividing the design domain into several layers. Xu et al. (Xu, Liu, Huang, Zou, and Ma, 2021) developed a multi-step algorithm to optimize the shell and interface layers for various optimized microstructures. Similar research work has also been conducted by Gu et al. (Gu, He, Dong, and Song, 2022), in which an improved ordered SIMP approach is developed to search the optimal layout of the coating and interface layers for multiple optimized microstructures. Jiang et al. (Jiang, Guo, Chen, Wei, Lei, and Gu, 2019) integrated the simultaneously optimized coated structure and microstructural topology via a conformal mapping technique and thus obtained a non-uniform lattice infilling for coated structures. Other studies use geometric components. For instance, Ngoc et al. (Ngoc, Hoang, and Lee, 2022) adapted a group of micro-solid bars for the representation of lattice infilling and updated certain parameters to achieve the layout of non-homogeneous microstructures under buckling criteria. Despite certain progress has been achieved, it should be noted that coated structures infilled with multiple microstructures are usually designed with several interfaces, when those density-based methods are implemented.

The connectivity between neighboring microstructures is a critical issue when multiple patterns of microstructures are considered for coated structures, which can greatly affect the effectiveness of load transfer and manufacturability, as shown in Fig. 5.1. To resolve this issue, Wang et al. (Wang and Kang, 2019) set non-design domains to force the connectivity between different microstructures. In the research of Du et al (Du, Zhou, Picelli, and Kim, 2018), a new measure named as connectivity index is introduced to evaluate the connectivity and further added as a constraint in the multiscale TO. Schury et al. (Schury, Stingl, and Wein, 2012) proposed the density tracking technique to ensure the microstructural connectivity. Duriez et al. (Duriez, Morlier, Charlotte, and Azzaro-Pantel, 2021) addressed the connectivity between neighboring microstructures through transmission zones of adaptive lengths defined on the edges of microstructures and developed a new efficient multiscale topology optimization framework. Recently, Matsui et al. (Matsui, Hoshiba, Kamada, Ogura, and Kato, 2023) proposed an enlarged connective region (ECR) method, in which two neighboring microstructures are grouped into a new microstructure and optimized considering the macroscale displacement of the enlarged connective region. Even though effective microstructural configurations can be achieved, the ECR method needs a pre-definition of macroscale domains for certain microstructures. Zhou et al. (Zhou and Li, 2008) developed three approaches to preserve the connectivity between neighboring microstructures, including connective constraint, pseudo load method, and unified formulation with nonlinear diffusion. Liu et al. (Liu, Kang, and Luo, 2020) presented a novel designable connective region (DCR) method and found the same material distribution within the connective regions of microstructures, thus the connectivity can be assured. Different from other methods, the DCR method requires no additional design variables or connectivity constraints, and has the compatibility to find the optimal macroscale distribution of multiple optimized microstructures.

The present study aims at proposing an effective multiscale density-based TO method for the

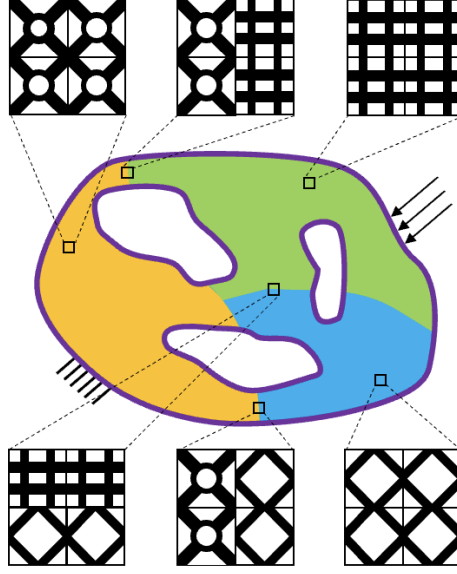


FIGURE 5.1: Connectivity between different microstructures within a coated structure.

design of coated structures with spatially varying microstructural infilling. Specifically, a new extended two-step filtering procedure is developed to distinguish the external coating and the porous inhomogeneous infilling, where a series of density filtering operations are used. At the macroscale, microstructures with different volume constraints can be regarded as different materials and the maximum volume fractions of them correspond to the design variables under the framework of the ordered SIMP method. The distribution of material blocks for microstructural configurations are initially identified via a novel piece-wise projection. After a special “strict” projection, the coating and its inner substrate can be separated using two-step filtered density fields. Meanwhile, the layout of varied microstructures within the coated structure can also be obtained. At the microscale level, the microstructural topologies are optimized using the SIMP method integrated with the numerical homogenization method (Hassani and Hinton, 1998). The designable connective region method is introduced to treat the connectivity issue, which is conveniently achieved via the microscale variable linking and no extra constraint is needed. As the iteration proceeds, material properties of the structures at two scales gradually stabilize and a coated structure infilled with multiple self-connected microstructures is thus obtained.

The remainder of this paper is arranged as follows. The modeling procedure of coated structures with multiple self-connected microstructural materials, a series of filtering operations, and the material interpolation functions at two scales are introduced in Section 5.2. Section 5.3 presents the TO formulation and the associated optimization procedure, along with sensitivity analyses for two scales described with details. Numerical examples are elaborated in Section 5.4 to test the proposed method, followed by conclusions drawn in Section 5.5.

5.2 Construction of the structural model

In this section, how to establish coated structures with multiple self-connected infilling microstructures will be presented at two scales. Generally, the model construction primarily consists of three parts, i.e., the identification of the external coating, the layout determination of macroscale material blocks for lattice materials, and the generation of multiple microstructures with great connectivity.

5.2.1 General idea

It is worth noting that designing a coated structure has been mature for density methods during the past two decades, however, how to optimize a coated structure with multiple infilling lattice materials relying on a single macroscale design variable field still needs to be studied. For a better understanding, the general idea of the model construction at two scales is illustrated in Fig. 5.2 using a coated structure infilled with three self-connected microstructures.

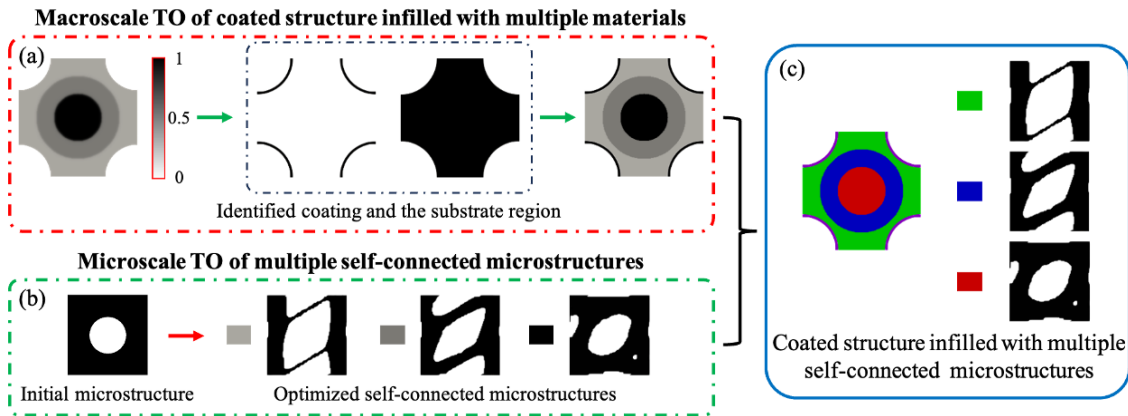


FIGURE 5.2: General idea for the model construction of coated structures with multiple self-connected lattice infilling microstructures.

At the macroscale, a density field that comprises several intermediate densities is used to detect the external coating and the substrate region for lattice infilling, as can be seen from the left part of Fig. 5.2(a). Specially, the coating is identified with desired uniform thickness with some filtering operations. After that, the macroscale geometrical model of a coated structure can be further constructed with infilling material blocks identified, described with certain intermediate densities. To achieve lightweight design and further improve structural performance, multiple types of microstructural configurations will be optimized from their initial microstructural guess with consideration of the geometrical connectivity between them. As presented in Fig. 5.2(b), each optimized lattice microstructural material will be used for certain material block of the coated structure and the optimization process of microstructures is simultaneously conducted with the evolution of their macroscale distribution. Finally, by combining the developed macrostructure

and multiple optimized microstructural configurations, the model of a coated structure infilled with multiple self-connected lattice microstructures can be constructed as presented in Fig. 5.2(c).

In the following subsections, the related filtering techniques used in the proposed method are described in detail and how to optimize self-connected microstructures for blocks of the substrate is also given.

5.2.2 Filters

Standard projection

Based on the tangent function, the standard projection proposed by Wang et al. (Wang, Lazarov, and Sigmund, 2011) is a filter which can effectively force the values within the interval $[0,1]$ towards either 0 or 1 and has been widely used in those density-based TO methods to get black-/white designs. Stated as in the following equation, this projection is used in the proposed approach on those filtered design variables during the two-step filtering operation.

$$\bar{x}_e^{\text{MA}} = \frac{\tanh(\beta_P \eta_P) + \tanh(\beta_P (x_e^{\text{MA}} - \eta_P))}{\tanh(\beta_P \eta_P) + \tanh(\beta_P (1 - \eta_P))}, \quad (e = 1, 2, \dots, n^{\text{MA}}), \quad (5.1)$$

where x_e^{MA} is the original elemental density; n^{MA} denotes the total number of macroscale elements. The standard projection effect is controlled by two parameters. The symbol β_P (representing β_{P_1} and β_{P_2} labeled in Fig. 5.5) determines the sharpness of the projection and the notion η_P (expressing parameters β_{P_1} and β_{P_2}) denotes the threshold value given between 0 and 1. When β_P tends to positive infinity, designs ($\bar{x}_e^{\text{MA}}$) are projected towards pure 0/1 solutions. Therefore, a small value of β_P is initially set and gradually increased via a parameter continuation process during the optimization for a better convergence behavior.

Piece-wise projection

Under the framework of the ordered SIMP method, macroscale material blocks of coated structures for different microstructures are described using certain intermediate element densities. In the proposed approach, the expected macroscale densities for the description of varied blocks are arranged in the ascending order of the normalized variable ρ_i^{MA} relying on ρ_i^{AO} . It should be noted that the void domains are also regarded as filled with a material with pretty low density. In this study, such a material for the void domain representation is set as $\rho_1^{\text{MA}} = 10^{-9}$ to avoid numerical singularity. The expression for the normalized macroscale density for separate microstructural topologies is defined as

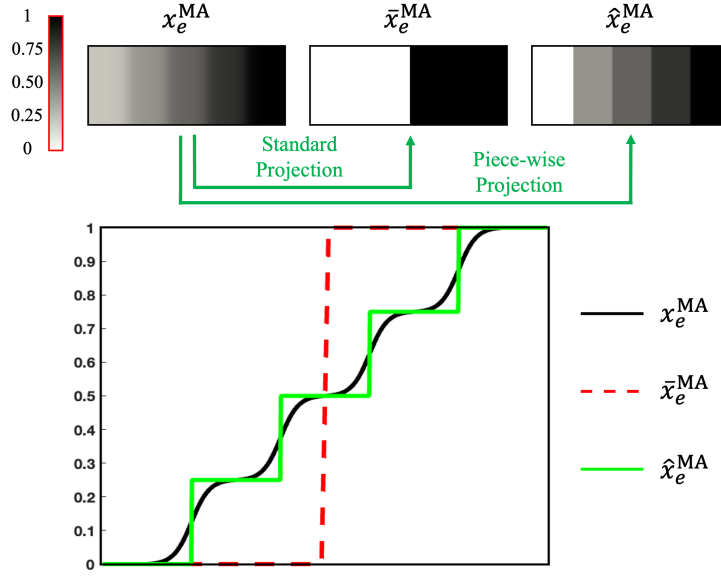


FIGURE 5.3: Comparison on the effect between the standard projection and the piece-wise projection. The notion x_e^{MA} represents $\tilde{\rho}_e^{\text{MA}}$ or $\tilde{\mu}_e^{\text{MA}}$, the symbol $\bar{x}_e^{\text{MA}}$ denotes μ^{MA} or φ^{MA} , and the mark $\hat{x}_e^{\text{MA}}$ relates to $\hat{\rho}_e^{\text{MA}}$.

$$\rho_i^{\text{MA}} = \frac{\rho_i^{\text{AO}}}{\rho_{\max}^{\text{MA}}}, \quad (i = 1, 2, \dots, m+1), \quad (5.2)$$

where ρ_i^{AO} equals to the ascending order of maximum volume fractions set on different microstructures; $\rho_{\max}^{\text{MA}}$ is the maximum of ρ_i^{AO} ; m equals to the number of considered microstructures. With Eq. (5.2), the macroscale density interval $[0,1]$ is then divided into m density intervals.

To make the intermediate macroscale design variables reach their certain normalized values ρ_i^{MA} , a piece-wise projection based on the standard projection Eq. (5.1) is introduced for producing different material blocks (Gu, He, Dong, and Song, 2022). For macroscale densities $x_e^{\text{MA}} \in [\rho_i^{\text{MA}}, \rho_{i+1}^{\text{MA}}]$, the projection is formulated as

$$\hat{x}_e^{\text{MA}} = \frac{\tanh(\beta_{\text{PP}}\eta_{\text{PP}}) + \tanh(\beta_{\text{PP}}(x_s^{\text{MA}} - \eta_{\text{PP}}))}{\tanh(\beta_{\text{PP}}\eta_{\text{PP}}) + \tanh(\beta_{\text{PP}}(1 - \eta_{\text{PP}}))} (\rho_{i+1}^{\text{MA}} - \rho_i^{\text{MA}}) + \rho_i^{\text{MA}}, \quad (5.3a)$$

$$(i = 1, 2, \dots, m; e = 1, 2, \dots, n^{\text{MA}}),$$

$$x_s^{\text{MA}} = \frac{x_e^{\text{MA}} - \rho_i^{\text{MA}}}{\rho_{i+1}^{\text{MA}} - \rho_i^{\text{MA}}}, \quad (i = 1, 2, \dots, m; e = 1, 2, \dots, n^{\text{MA}}), \quad (5.3b)$$

where $\hat{x}_e^{\text{MA}}$ is the piece-wisely projected density field; β_{PP} and η_{PP} are the sharpness parameter and the threshold parameter, respectively. Actually, the piece-wise projection Eq. (5.3) can be deemed as performing the standard projection filter in each density interval, in which the intermediate densities within the intervals are projected towards ρ_i^{MA} and ρ_{i+1}^{MA} under the effect of β_{PP} and

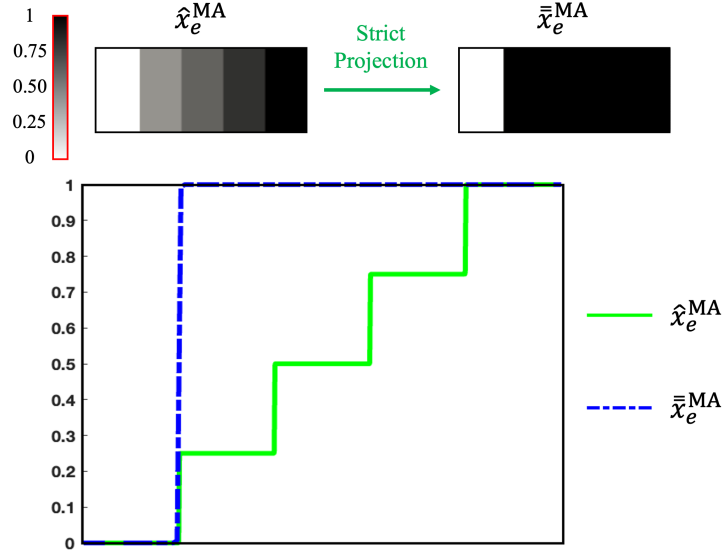


FIGURE 5.4: Effect of the strict projection. The symbol $\bar{x}_e^{MA}$ indicates ρ_S^{MA} in Fig. 5.5.

η_{PP} . For a better illustration, the comparison between the standard projection and the piece-wise projection is presented in Fig. 5.3.

Strict projection

The main idea of the strict projection is to detect those subdomains with solid material distribution over the whole design domain. Based on this concept and the multi-material description of the ordered SIMP method using intermediate density values between 0 and 1, the strict projection has no theoretical difference with the standard projection but owns a smaller threshold value η_{SP} (which should not be larger than ρ_2^{MA} for a correct detection). Under the control of β_{SP} and η_{SP} , the piece-wisely projected density field is then modified as a pure 0/1 variable field, judging whether a point in the design domain has material or not. The effect of the strict projection is given in Fig. 5.4 to offer a more intuitive explanation. After obtaining the material/void judgment field, the problem is temporarily transformed as the pure coating identification issue as studied in those existing research work and the classical two-step filtering operation can then be implemented.

Smoothing filter

In order to realize the smoothing, a Helmholtz-type partial differential equation-based PDE filter is introduced (Lazarov and Sigmund, 2011). For the density field $\mathbf{X}^{MA}$, its filtered density field $\tilde{\mathbf{X}}^{MA}$ is implicitly defined as the solution of the following equation.

$$-r^2 \nabla^2 \tilde{\mathbf{X}}^{MA} + \tilde{\mathbf{X}}^{MA} = \mathbf{X}^{MA}, \quad (5.4)$$

where the notation r is a length scale parameter; $\tilde{\mathbf{X}}^{\text{MA}}$ represents $\tilde{\rho}_s^{\text{MA}}$ and $\tilde{\mu}^{\text{MA}}$, and $\mathbf{X}^{\text{MA}}$ denotes ρ_s^{MA} and μ^{MA} . The Helmholtz smoothing filter radius R (representing R_{S_1} and R_{S_2}) can be determined by the length scale parameter r via the following relationship:

$$R = 2\sqrt{3}r. \quad (5.5)$$

5.2.3 Extended two-step filtering procedure for coated structures infilled with multiple lattice materials

Taking a coated structure involving three lattice infilling materials as an example, Fig. 5.5 illustrates an overview of the conceptual design procedure and the detailed roadmap developed in this research. Different from other research works (Bai and Zuo, 2022; Gan and Wang, 2021), only one macroscale design variable field is utilized in the developed approach for the construction of coated structures infilled with multiple lattice materials.

As shown in the left of Fig. 5.5, the spatial layout of multiple microstructural blocks at the macroscale is initially defined via a piece-wise projection based on the initial density field ρ^{MA} and generates a new field $\hat{\rho}^{\text{MA}}$, which is prepared for the latter multi-material infilling determination. It should be noted that each density value in the $\hat{\rho}^{\text{MA}}$ field corresponds to a specific optimized microstructure. Then, a strict projection is performed to detect the material layout area of the current iteration step and a projected field ρ_s^{MA} is obtained. With such an operation, the problem is subsequently transformed as the pure coating-infilling identification study and the classical two-step filtering approach is implemented to distinguish the coating and the substrate. Compared to the research works made by Groen et al (Groen, Wu, and Sigmund, 2019), no gradient calculation is needed in the presented study and thus simplify the whole filtering procedure. To be specific, as presented in the right of Fig. 5.5, mixtures of two sets of variables, i.e. μ^{MA} and ϕ^{MA} , are conducted, respectively yielding the coating identification field and the establishment of the substrate, and thus the coated structure is constructed. Finally, the previously prepared field $\hat{\rho}^{\text{MA}}$ is assembled to the coated structure by simply multiplying it with the substrate field, leading to the multi-material microstructural infilling (depicted with varied colors in Fig. 5.5) for coated structures. Also, the thickness of the external coating can be defined indirectly by setting the filter radius for the second filtering operation in the two-step filtering.

5.2.4 Designable connective region method for self-connected microstructures

In this study, the substrate of coated structures we plan to design are composed of multiple types of microstructures. However, as already mentioned in the introduction, the optimized multiple microstructures may not be well-connected and thus cannot be manufactured in practice by the AM technique. To deal with this necessary issue, the DCR method (a density-based method

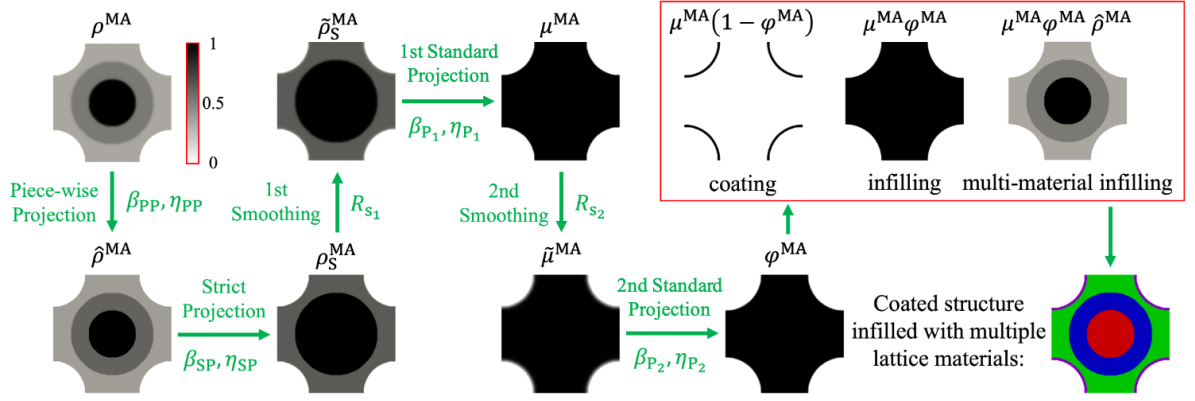


FIGURE 5.5: The extended two-step filtering procedure for the construction of coated structures infilled with multiple lattice materials.

proposed by Liu et al. (Liu, Kang, and Luo, 2020)) is introduced into the proposed concurrent multiscale TO approach to achieve self-connected microstructural configurations. For a coated structure considering m lattice microstructures, the DCR method divides the design domain of all m microstructures into two parts, i.e., designable connective region and the non-connective region. The thickness of the connective region is defined by a parameter T_c and can be set with different values in varied directions. As schematically illustrated in Fig. 5.6, the designable connective region (marked in blue) of 2D square-shaped microstructures is defined around the four edges of unit cells, where the microscale densities located in designable connective regions of varied microstructures share the same value via the design variable linking. For the q -th and g -th lattice microstructures, the design variable linking is constructed as the following equation:

$$\rho_{qt}^{MI} = \rho_{gt}^{MI}, \quad (q, g = 1, 2, \dots, m; t = 1, 2, \dots, n_c), \quad (5.6)$$

where n_c is the total number of elements in the designable connective region.

For microscale elements in the non-connective region, their design variables are re-indexed from $\rho_{q(n_c+1)}^{MI}$ to $\rho_{qn^{MI}}^{MI}$, where n^{MI} is the total number of elements within a unit cell.

With Eq. (5.6) and a filter radius smaller than the thickness of the connective region, all of the considered microstructural configurations have the same topology over the connective region during the optimization process, which is simultaneously optimized with the material distribution in the non-designable region. Therefore, the connectivity between neighbouring microstructures is greatly ensured and the interaction of density evolution in different regions of unit cells can be well considered. The DCR method is easy to implement for the design of multiple microstructures and no additional design variable, evaluation index, or constraint is needed.

Although many other shapes of elements can be selected, such as hexagon elements, we only consider square unit cells for 2D microstructures in the presented study.

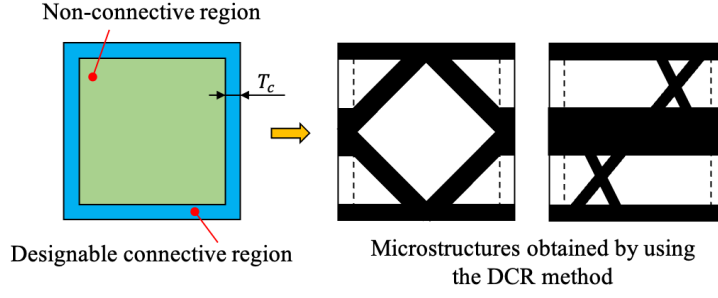


FIGURE 5.6: Illustration of how the designable connective region method ensures the microstructural connectivity.

5.2.5 Material interpolation functions

Homogenization method for microstructures

In the proposed concurrent multiscale TO approach, the separation of scales is used, where the size of a microstructure is pretty small in comparison with that of its subdomain at the macroscale, and each subdomain for different lattice materials is filled with the periodically arrangement of a certain optimized microstructural configuration. Thus, the equivalent material properties of lattice material microstructures can be computed with the homogenization method, which is sufficiently effective for bridging the optimization at two scales. Using the asymptotic homogenization method, the calculation of the equivalent elasticity tensor of the q -th lattice microstructure is formulated as

$$\mathbf{D}_q^H = \frac{1}{|\mathbf{Y}|} \sum_{j=1}^{n^{\text{MI}}} \int_{\mathbf{Y}_j} \left(\boldsymbol{\varepsilon}^0 - \boldsymbol{\varepsilon}^* \left(\boldsymbol{\chi}_q \right) \right)^T \mathbf{D}_{qj}^{\text{MI}} \left(\boldsymbol{\varepsilon}^0 - \boldsymbol{\varepsilon}^* \left(\boldsymbol{\chi}_q \right) \right) d\mathbf{y}, \quad (5.7)$$

where $|\mathbf{Y}|$ is the area of a unit cell; $\boldsymbol{\varepsilon}^0$ corresponds to the linearly independent test strain fields, where 3 load cases should be considered for 2D microstructures; $\boldsymbol{\varepsilon}^*(\boldsymbol{\chi})$ indicates the unknown strain field in the unit cell, induced by the characteristic displacement field $\boldsymbol{\chi}_q$; $\mathbf{D}_{qj}^{\text{MI}}$ is the elasticity tensor of the element j in the q -th microstructure, which can be expressed as

$$\mathbf{D}_{qj}^{\text{MI}} = \left[\left(\rho_{qj}^{\text{MI}} \right)^p \cdot \left(E_s^{\text{MI}} - E_0^{\text{MI}} \right) + E_0^{\text{MI}} \right] \cdot \mathbf{D}_0^{\text{MI}}, \quad (j = 1, 2, \dots, n_c, n_c + 1, \dots, n^{\text{MI}}), \quad (5.8)$$

where ρ_{qj}^{MI} is the density value of the element qj ; p is the penalization parameter; E_s^{MI} and E_0^{MI} are the Young's modulus of the solid and void materials at the microscale, respectively; $\mathbf{D}_0^{\text{MI}}$ is the elasticity tensor of the base microstructural material, which is formulated as

$$\mathbf{D}_0^{\text{MI}} = \frac{1}{1 - (v_0^{\text{MI}})^2} \begin{bmatrix} 1 & v_0^{\text{MI}} & 0 \\ v_0^{\text{MI}} & 1 & 0 \\ 0 & 0 & \frac{1-v_0^{\text{MI}}}{2} \end{bmatrix}, \quad (5.9)$$

in which v_0^{MI} is the Poisson's ratio of the base material at the microscale.

The unknown strain field $\boldsymbol{\varepsilon}^*(\boldsymbol{\chi})$ can be obtained by solving the following microscale equation under the periodic boundary condition:

$$\sum_{j=1}^{n^{\text{MI}}} \int_{\mathbf{Y}_j} \boldsymbol{\varepsilon}(\boldsymbol{\delta})^T \mathbf{D}_{q_j}^{\text{MI}} [\boldsymbol{\varepsilon}^0 - \boldsymbol{\varepsilon}^*(\boldsymbol{\chi}_q)] \, d\mathbf{y} = 0, \quad \forall \boldsymbol{\delta} \in U(\mathbf{Y}), \quad (5.10)$$

where $\boldsymbol{\delta}$ is the virtual displacement field and $U(\mathbf{Y})$ is the set of all the kinematically admissible displacements in $\mathbf{Y}$.

Material interpolation scheme at macroscale

In the proposed approach, the macroscale TO on the distribution of multiple material blocks for various microstructures is conducted relying on the ordered SIMP method, which is an effective multi-material TO method with no additional design variables needed. Introducing the scaling coefficient $\mathbf{A}_D$ and the translation coefficient $\mathbf{B}_D$, the ordered SIMP interpolation of the elasticity tensor of an element $\hat{\rho}_e^{\text{MA}}$ is formulated as

$$\mathbf{D}(\hat{\rho}_e^{\text{MA}}) = \mathbf{A}_D \cdot (\hat{\rho}_e^{\text{MA}})^p + \mathbf{B}_D, \quad (e = 1, 2, \dots, n^{\text{MA}}). \quad (5.11)$$

After the piece-wise projection Eq. (5.3), if the macroscale density $\hat{\rho}_e^{\text{MA}} \in [\rho_i^{\text{MA}}, \rho_{i+1}^{\text{MA}}]$, the coefficients $\mathbf{A}_D$ and $\mathbf{B}_D$ are respectively defined as following formulations:

$$\mathbf{A}_D = \frac{\mathbf{D}_i^H - \mathbf{D}_{i+1}^H}{(\rho_i^{\text{MA}})^p - (\rho_{i+1}^{\text{MA}})^p}, \quad (i = 1, 2, \dots, m), \quad (5.12a)$$

$$\mathbf{B}_D = \mathbf{D}_i^H - \mathbf{A}_D (\rho_i^{\text{MA}})^p, \quad (i = 1, 2, \dots, m). \quad (5.12b)$$

In this subsection, the stiffness and volume interpolation functions of the material model are created. As introduced before, the macroscale coated structure in this paper is constructed based on $\boldsymbol{\mu}^{\text{MA}}$, $\boldsymbol{\varphi}^{\text{MA}}$, and $\hat{\boldsymbol{\rho}}^{\text{MA}}$ fields. After the first filtering operation of the classical two-step filtering procedure, an erosion is implemented on the density field $\boldsymbol{\mu}^{\text{MA}}$ with a larger threshold value $\eta_{P_2} = 0.5 + \Delta\eta_{P_2}$ (where $\Delta\eta_{P_2} \in (0, 0.5)$), yielding a modified density field $\boldsymbol{\varphi}^{\text{MA}}$. Subsequently, the outer coating and the substrate region of a coated structure can be distinguished through the different and common parts between the fields $\boldsymbol{\mu}^{\text{MA}}$ and $\boldsymbol{\varphi}^{\text{MA}}$ with a simple algebraic calculation. In particular, the external coating is found when $\mu_e^{\text{MA}} = 1$ and $\varphi_e^{\text{MA}} = 0$, and the domain for multiple lattice microstructures is determined by $\mu_e^{\text{MA}} = \varphi_e^{\text{MA}} = 1$. Therefore, the elastic tensor matrix of a coated structure infilled with lattice microstructures is composed of the elasticity tensor of the external coating $\mathbf{D}_{\text{coating}}$ and the one of the multi-material infilling $\mathbf{D}_{\text{infilling}}$, expressed as

$$\begin{aligned} \mathbf{D}^{\text{MA}} &= \mathbf{D}_{\text{coating}} + \mathbf{D}_{\text{infilling}} \\ &= (\boldsymbol{\mu}^{\text{MA}})^p \left[1 - (\boldsymbol{\varphi}^{\text{MA}})^p \right] \cdot \mathbf{D}_{\text{coating}} + (\boldsymbol{\mu}^{\text{MA}})^p (\boldsymbol{\varphi}^{\text{MA}})^p \left[\mathbf{A}_D \cdot (\hat{\boldsymbol{\rho}}^{\text{MA}})^p + \mathbf{B}_D \right], \end{aligned} \quad (5.13)$$

where, the term $\mathbf{D}_{\text{coating}}$ in the above expression can be formulated as the following equation:

$$\begin{aligned}\mathbf{D}_{\text{coating}} &= E_s^{\text{MA}} \cdot \mathbf{D}_0^{\text{MA}} \\ &= \frac{E_s^{\text{MA}}}{1 - (v_0^{\text{MA}})^2} \begin{bmatrix} 1 & v_0^{\text{MA}} & 0 \\ v_0^{\text{MA}} & 1 & 0 \\ 0 & 0 & \frac{1-v_0^{\text{MA}}}{2} \end{bmatrix},\end{aligned}\quad (5.14)$$

in which E_s^{MA} and v_0^{MA} are the Young's modulus and Poisson's ratio of the macroscale base material, respectively.

With the radius filter R_{S_2} for the second filtering operation, it should be noted that the thickness of the external coating ω can be controlled by the following formulation when the parameter $\Delta\eta_{P_2}$ is given as 0.45.

$$\omega \approx 1.5R_{S_2}. \quad (5.15)$$

For analytical details of the above equation, readers can be referred to the research of Luo et al (Luo, Li, and Liu, 2019).

Because of the lattice microstructures as the infilling, the real volume of the microstructural infilling should be calculated with consideration of the real volume fractions of different microstructures. This can be easily achieved in the proposed TO framework since the normalized macroscale density ρ_i^{MA} for varied types of microstructures is set by using their maximum volume fractions based on Eq. (5.2). Therefore, by multiplying the term $\rho_{\text{max}}^{\text{MA}}$, the volume of the macroscale coated structure infilled with multiple microstructures over the design domain Ω can be accurately calculated as

$$\begin{aligned}V^{\text{MA}} &= V_{\text{coating}} + V_{\text{infilling}} \\ &= \int_{\Omega} \mu^{\text{MA}} [1 - \phi^{\text{MA}}] dx + \int_{\Omega} \mu^{\text{MA}} \phi^{\text{MA}} \hat{\rho}^{\text{MA}} \rho_{\text{max}}^{\text{MA}} dx.\end{aligned}\quad (5.16)$$

5.3 Concurrent multiscale topology optimization

5.3.1 Problem formulation

The optimization target in this paper is to minimize the static compliance of coated structures by concurrently optimizing structures at two scales. Specifically, topologies of multiple self-connected microstructures are iteratively updated with the evolution of their spatial distribution within the gradually optimized macroscale coated structure. Besides, only one kind of material is utilized for structures at two scales, thus, the effect of a total volume constraint works the same as the mass constraint in the proposed approach. With the calculation of the exact volume of the coated structure, a macroscale volume constraint is introduced to limit the total material consumption. At the microscale, each lattice microstructure corresponds to a certain density field

$\rho_i^{\text{MA}} (i = 2, 3, \dots, m)$ and totally $(m - 1)$ microstructural maximum volume fractions are considered. Therefore, the mathematical model for the optimization problem can be formulated as

$$\begin{aligned}
& \text{find: } \rho_e^{\text{MA}}, \rho_{ij}^{\text{MI}} \\
& \quad \left(e = 1, 2, \dots, n^{\text{MA}}; i = 1, 2, \dots, m; j = 1, 2, \dots, n_c, n_c + 1, \dots, n^{\text{MI}} \right), \\
& \text{min: } c = \left(\boldsymbol{\varepsilon}^{\text{MA}} \right)^T \mathbf{D}^{\text{MA}} \boldsymbol{\varepsilon}^{\text{MA}}, \\
& \text{s.t.: } \mathbf{a}(\mathbf{u}^{\text{MA}}, \mathbf{v}^{\text{MA}}) = \mathbf{l}(\mathbf{v}^{\text{MA}}), \quad \forall \mathbf{v}^{\text{MA}} \in U^{\text{MA}}, \\
& \quad G^{\text{MA}} = V^{\text{MA}} / |\boldsymbol{\Omega}| - f^{\text{MA}} \leq 0, \\
& \quad G_i^{\text{MI}} = V_i^{\text{MI}} / |\mathbf{Y}| - f_i^{\text{MI}} \leq 0, \quad (i = 1, 2, \dots, m), \\
& \quad \rho_{qt}^{\text{MI}} = \rho_{gt}^{\text{MI}}, \quad (q, g = 1, 2, \dots, m; t = 1, 2, \dots, n_c), \\
& \quad 0 < \rho_{\min}^{\text{MA}} \leq \rho_e^{\text{MA}} \leq 1, \quad (e = 1, 2, \dots, n^{\text{MA}}), \\
& \quad 0 < \rho_{\min}^{\text{MI}} \leq \rho_{ij}^{\text{MI}} \leq 1, \quad (i = 1, 2, \dots, m; j = 1, 2, \dots, n^{\text{MI}}),
\end{aligned} \tag{5.17}$$

where c is the static compliance; $\boldsymbol{\varepsilon}^{\text{MA}}$ represents the macroscale strain of the coated structure; G^{MA} and G^{MI} are the macroscale and microscale volume constraints, respectively; V^{MA} is the macroscale structural volume, while V_i^{MI} is the structural volume of the i -th microstructure; $|\boldsymbol{\Omega}|$ is the volume of the macroscale design domain; f^{MA} and f_i^{MI} are the given maximum volume fractions for two scales; ρ_{ij}^{MA} and ρ_{ij}^{MI} are the lower limits for design variables at two scales; $\mathbf{u}^{\text{MA}}$ is the macroscale structural displacement field and $\mathbf{v}^{\text{MA}}$ describes the kinematically admissible virtual displacement field; U^{MA} is the space of admissible virtual displacement field. The energy bilinear form $\mathbf{a}(\mathbf{u}^{\text{MA}}, \mathbf{v}^{\text{MA}})$ and the load linear form $\mathbf{l}(\mathbf{v}^{\text{MA}})$ are respectively formulated as

$$\mathbf{a}(\mathbf{u}^{\text{MA}}, \mathbf{v}^{\text{MA}}) = \int_{\boldsymbol{\Omega}} (\boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{u}^{\text{MA}}))^T \cdot \mathbf{D}^{\text{MA}} \cdot \boldsymbol{\varepsilon}^{\text{MA}}(\mathbf{v}^{\text{MA}}) d\boldsymbol{\Omega}, \tag{5.18a}$$

$$\mathbf{l}(\mathbf{v}^{\text{MA}}) = \int_{\boldsymbol{\Omega}} \mathbf{f} \cdot \mathbf{v}^{\text{MA}} d\boldsymbol{\Omega} + \int_{\Gamma_N} \mathbf{t} \cdot \mathbf{v}^{\text{MA}} d\Gamma, \tag{5.18b}$$

where $\mathbf{f}$ is the body force and $\mathbf{t}$ is the surface traction applied on the Neumann boundary.

5.3.2 Optimization procedure

The flowchart of the numerical procedure for solving the concurrent multiscale TO problem using the proposed approach is illustrated in Fig. 5.7, and the detail explanation is given as follows:

1. Define the designable connective region and non-designable region for the connectivity issue between different microstructures.
2. Initialize the macrostructure and multiple microstructures. Calculate the normalized densities for varied microstructural description via Eq. (5.2) and set other design parameters

needed in the proposed method.

3. Carry out finite element (FE) analysis at the microscale and evaluate the homogenized elasticity tensor $\mathbf{D}_q^H$ of multiple microstructures by using the homogenization method (Eq. (5.7)).
4. Construct the material model of the coated structure. Firstly, the separation of the coating is achieved and multiple material blocks for self-connected infilling microstructures are identified using the developed extended two-step filtering procedure shown in Fig. 5.5. Secondly, the elasticity tensor and the volume of the macrostructure are respectively interpolated via Eqs. (5.13) and (5.16).
5. Perform FE analysis at the macroscale and then calculate the objective function value and constraints.
6. Check whether the convergence criteria are satisfied. If yes, the optimization is finished and the final coated structure and its optimized self-connected multiple infilling microstructures are obtained; If no, continue to Step (7).
7. Calculate the macroscale and microscale sensitivities of the objective function and constraints.
8. Update design variables at two scales via the Method of Moving Asymptotes (MMA) (Svanberg, 1987) optimizer.
9. Return back to Step (3) and repeat the optimization procedure.

5.3.3 Sensitivity analysis

In this paper, the design variables at two scales are concurrently optimized using the MMA algorithm. Thus, sensitivities of the static compliance and volume constraints need to be numerically derived.

Macroscale sensitivity analysis

According to the self-adjoint of the optimization problem, the static compliance with respect to the macroscale design variable can be derived as the following equation:

$$\frac{\partial c}{\partial \rho_e^{\text{MA}}} = \left(\boldsymbol{\epsilon}^{\text{MA}} \right)^T \frac{\partial \mathbf{D}^{\text{MA}}}{\partial \rho_e^{\text{MA}}} \boldsymbol{\epsilon}^{\text{MA}}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \quad (5.19)$$

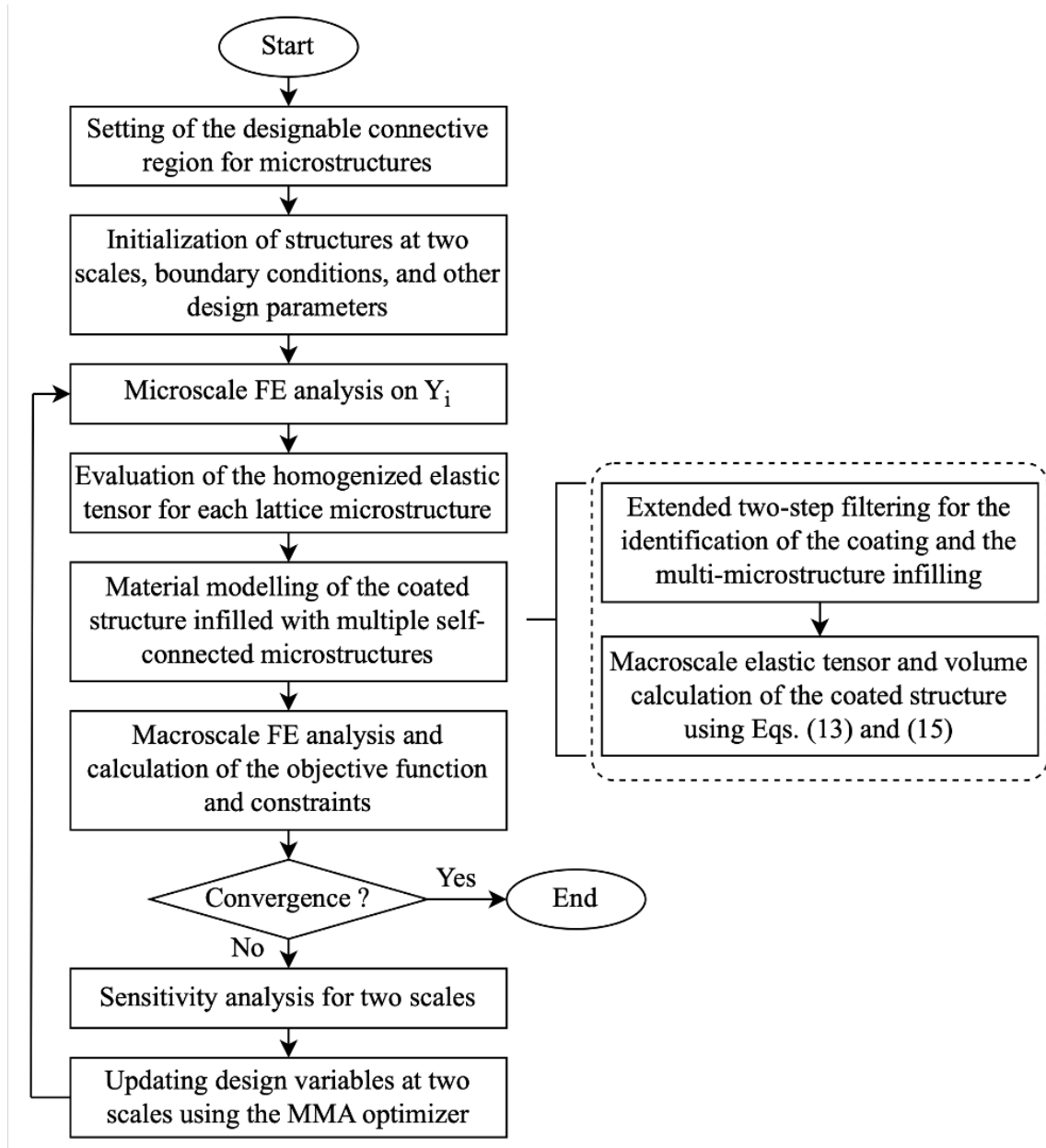


FIGURE 5.7: Flowchart of the multiscale optimization procedure.

Based on the elasticity tensor interpolation Eq. (5.13), the term $\frac{\partial \mathbf{D}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}$ in the above equation can be derived using the product rule as follows:

$$\begin{aligned} \frac{\partial \mathbf{D}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} &= p \cdot (\mu_e^{\text{MA}})^{p-1} \cdot \left\{ (\varphi_e^{\text{MA}})^p \left[\mathbf{A}_D \cdot (\hat{\rho}_e^{\text{MA}})^p + \mathbf{B}_D \right] + \left[1 - (\varphi_e^{\text{MA}})^p \right] \cdot \mathbf{D}_{\text{coating}} \right\} \frac{\partial \mu_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} \\ &+ \left[(\mu_e^{\text{MA}})^p \cdot p \cdot (\varphi_e^{\text{MA}})^{p-1} \cdot \mathbf{A}_D \cdot (\hat{\rho}_e^{\text{MA}})^p + p \cdot (\varphi_e^{\text{MA}})^{p-1} \cdot \mathbf{B}_D - p \cdot (\varphi_e^{\text{MA}})^{p-1} \cdot \mathbf{D}_{\text{coating}} \right] \frac{\partial \varphi_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} \\ &+ (\mu_e^{\text{MA}})^p \cdot (\varphi_e^{\text{MA}})^p \cdot \mathbf{A}_D \cdot p \cdot (\hat{\rho}_e^{\text{MA}})^{p-1} \frac{\partial \hat{\rho}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \end{aligned} \quad (5.20)$$

Using the chain rule, the term $\frac{\partial \mu_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}$ in the above expression is elaborated as

$$\frac{\partial \mu_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} = \frac{\partial \mu_e^{\text{MA}}}{\partial \tilde{\rho}_{s_e}^{\text{MA}}} \frac{\partial \tilde{\rho}_{s_e}^{\text{MA}}}{\partial \rho_{s_e}^{\text{MA}}} \frac{\partial \rho_{s_e}^{\text{MA}}}{\partial \hat{\rho}_e^{\text{MA}}} \frac{\partial \hat{\rho}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \quad (5.21)$$

Similarly, with substitution of Eq. (5.21), the term $\frac{\partial \varphi_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}$ can also be obtained using the chain rule as

$$\begin{aligned} \frac{\partial \varphi_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} &= \frac{\partial \varphi_e^{\text{MA}}}{\partial \tilde{\mu}_e^{\text{MA}}} \frac{\partial \tilde{\mu}_e^{\text{MA}}}{\partial \mu_e^{\text{MA}}} \frac{\partial \mu_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} \\ &= \frac{\partial \varphi_e^{\text{MA}}}{\partial \tilde{\mu}_e^{\text{MA}}} \frac{\partial \tilde{\mu}_e^{\text{MA}}}{\partial \mu_e^{\text{MA}}} \frac{\partial \mu_e^{\text{MA}}}{\partial \tilde{\rho}_{s_e}^{\text{MA}}} \frac{\partial \tilde{\rho}_{s_e}^{\text{MA}}}{\partial \rho_{s_e}^{\text{MA}}} \frac{\partial \rho_{s_e}^{\text{MA}}}{\partial \hat{\rho}_e^{\text{MA}}} \frac{\partial \hat{\rho}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \end{aligned} \quad (5.22)$$

According to the Standard projection Eq. (5.1), the partial derivatives $\frac{\partial \mu_e^{\text{MA}}}{\partial \tilde{\rho}_e^{\text{MA}}}$ and $\frac{\partial \varphi_e^{\text{MA}}}{\partial \tilde{\mu}_e^{\text{MA}}}$ can be respectively calculated as

$$\frac{\partial \mu_e^{\text{MA}}}{\partial \tilde{\rho}_{s_e}^{\text{MA}}} = \beta_{P_1} \frac{1 - \tanh^2(\beta_{P_1}(\tilde{\rho}_{s_e}^{\text{MA}} - \eta_{P_1}))}{\tanh(\beta_{P_1}\eta_{P_1}) + \tanh(\beta_{P_1}(1 - \eta_{P_1}))}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \quad (5.23)$$

$$\frac{\partial \varphi_e^{\text{MA}}}{\partial \tilde{\mu}_e^{\text{MA}}} = \beta_{P_2} \frac{1 - \tanh^2(\beta_{P_2}(\tilde{\mu}_e^{\text{MA}} - \eta_{P_2}))}{\tanh(\beta_{P_2}\eta_{P_2}) + \tanh(\beta_{P_2}(1 - \eta_{P_2}))}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \quad (5.24)$$

Associated with the Piece-wise projection Eq. (5.3), the calculation of $\frac{\partial \hat{\rho}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}$ is written as the following equation if $\rho_e^{\text{MA}} \in [\rho_i^{\text{MA}}, \rho_{i+1}^{\text{MA}}]$.

$$\frac{\partial \hat{\rho}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} = \beta_{PP} \frac{1 - \tanh^2(\beta_{PP}(\rho_b^{\text{MA}} - \eta_{PP}))}{\tanh(\beta_{PP}\eta_{PP}) + \tanh(\beta_{PP}(1 - \eta_{PP}))}, \quad (e = 1, 2, \dots, n^{\text{MA}}), \quad (5.25a)$$

$$\rho_b^{\text{MA}} = \frac{\rho_e^{\text{MA}} - \rho_i^{\text{MA}}}{\rho_{i+1}^{\text{MA}} - \rho_i^{\text{MA}}}, \quad (i = 1, 2, \dots, m; e = 1, 2, \dots, n^{\text{MA}}). \quad (5.25b)$$

As for the term $\frac{\partial \rho_{s_e}^{\text{MA}}}{\partial \hat{\rho}_e^{\text{MA}}}$, it can be obtained based on Eq. (5.24) by replacing the corresponding parameters and variables, due to the similarity between the Standard projection and the Strict projection.

Next, the sensitivity of the macroscale volume constraint with respect to macroscale design variables can be calculated in the same way by

$$\begin{aligned} \frac{\partial V^{\text{MA}}}{\partial \rho_e^{\text{MA}}} &= \left(1 - \varphi_e^{\text{MA}} + \varphi_e^{\text{MA}} \hat{\rho}_e^{\text{MA}} \rho_{\max}\right) \frac{\partial \mu_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} \\ &\quad + \left(\mu_e^{\text{MA}} \hat{\rho}_e^{\text{MA}} \rho_{\max} - \mu_e^{\text{MA}}\right) \frac{\partial \varphi_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}} \\ &\quad + \mu_e^{\text{MA}} \hat{\rho}_e^{\text{MA}} \rho_{\max} \frac{\partial \hat{\rho}_e^{\text{MA}}}{\partial \rho_e^{\text{MA}}}, \quad (e = 1, 2, \dots, n^{\text{MA}}). \end{aligned} \quad (5.26)$$

Microscale sensitivity analysis

Similarly, the sensitivity analysis of the objective function with respect to the microscale design variable ρ_{ij}^{MI} can be formulated as follows:

$$\frac{\partial c}{\partial \rho_{ij}^{\text{MI}}} = - \left(\boldsymbol{\varepsilon}^{\text{MA}}\right)^{\text{T}} \frac{\partial \mathbf{D}^{\text{MA}}}{\partial \rho_{ij}^{\text{MI}}} \boldsymbol{\varepsilon}^{\text{MA}}, \quad (i = 1, 2, \dots, m; j = 1, 2, \dots, n^{\text{MI}}), \quad (5.27)$$

where the term $\frac{\partial \mathbf{D}^{\text{MA}}}{\partial \rho_{ij}^{\text{MI}}}$ is calculated as

$$\frac{\partial \mathbf{D}^{\text{MA}}}{\partial \rho_{ij}^{\text{MI}}} = \left(\boldsymbol{\mu}^{\text{MA}}\right)^p \left(\boldsymbol{\varphi}^{\text{MA}}\right)^p \left[\frac{\partial \mathbf{A}_{\text{D}}}{\partial \rho_{ij}^{\text{MI}}} \left(\hat{\rho}_e^{\text{MA}}\right)^p + \frac{\partial \mathbf{B}_{\text{D}}}{\partial \rho_{ij}^{\text{MI}}} \right], \quad (i = 1, 2, \dots, m; j = 1, 2, \dots, n^{\text{MI}}). \quad (5.28)$$

In the proposed concurrent multiscale TO method, it should be emphasized that the i -th lattice microstructure affects the elasticity tensor of the $(i - 1)$ -th and $(i + 1)$ -th microstructures. Therefore, a two-case discussion should be conducted when calculating the sensitivity terms $\frac{\partial \mathbf{A}_{\text{D}}}{\partial \rho_{ij}^{\text{MI}}}$ and $\frac{\partial \mathbf{B}_{\text{D}}}{\partial \rho_{ij}^{\text{MI}}}$. Besides, due to the introduction of the DCR method and the design variable linking over the designable connective region ($\rho_{1j}^{\text{MI}} = \rho_{2j}^{\text{MI}} = \dots = \rho_{mj}^{\text{MI}}$), sensitivities with respect to the microscale design variables should also be derived in different ways.

For those microscale elements within the non-connective region, terms $\frac{\partial \mathbf{A}_{\text{D}}}{\partial \rho_{ij}^{\text{MI}}}$ and $\frac{\partial \mathbf{B}_{\text{D}}}{\partial \rho_{ij}^{\text{MI}}}$ can be formulated as the following equation when $\hat{\rho}_e^{\text{MA}} \in [\rho_i^{\text{MA}}, \rho_{i+1}^{\text{MA}}]$, according to Eqs. (5.12a) and (5.12b).

$$\frac{\partial \mathbf{A}_D}{\partial \rho_{ij}^{\text{MI}}} = \frac{1}{(\rho_i^{\text{MA}})^p - (\rho_{i+1}^{\text{MA}})^p} \frac{\partial \mathbf{D}_i^{\text{H}}}{\partial \rho_{ij}^{\text{MI}}}, \quad (i = 1, 2, \dots, m; j = n_c + 1, n_c + 2, \dots, n^{\text{MI}}). \quad (5.29a)$$

$$\frac{\partial \mathbf{B}_D}{\partial \rho_{ij}^{\text{MI}}} = \frac{\partial \mathbf{D}_i^{\text{H}}}{\partial \rho_{ij}^{\text{MI}}} - \frac{\partial \mathbf{A}_D}{\partial \rho_{ij}^{\text{MI}}} (\rho_i^{\text{MA}})^p, \quad (i = 1, 2, \dots, m; j = n_c + 1, n_c + 2, \dots, n^{\text{MI}}). \quad (5.29b)$$

When $\hat{\rho}_e^{\text{MA}} \in [\rho_{i-1}^{\text{MA}}, \rho_i^{\text{MA}}]$, the above expressions are modified as

$$\frac{\partial \mathbf{A}_D}{\partial \rho_{ij}^{\text{MI}}} = -\frac{1}{(\rho_{i-1}^{\text{MA}})^p - (\rho_i^{\text{MA}})^p} \frac{\partial \mathbf{D}_i^{\text{H}}}{\partial \rho_{ij}^{\text{MI}}}, \quad (i = 2, 3, \dots, m+1; j = n_c + 1, n_c + 2, \dots, n^{\text{MI}}). \quad (5.30a)$$

$$\frac{\partial \mathbf{B}_D}{\partial \rho_{ij}^{\text{MI}}} = -\frac{\partial \mathbf{A}_D}{\partial \rho_{ij}^{\text{MI}}} (\rho_{i-1}^{\text{MA}})^p, \quad (i = 2, 3, \dots, m+1; j = n_c + 1, n_c + 2, \dots, n^{\text{MI}}). \quad (5.30b)$$

As for a microscale element within the designable connective region, i.e., $\rho_j^{\text{MI}} (j = 1, 2, \dots, n_c)$, its sensitivity calculation should consider the information of all the lattice microstructures. Therefore, when $\hat{\rho}_e^{\text{MA}} \in [\rho_i^{\text{MA}}, \rho_{i+1}^{\text{MA}}]$, $\frac{\partial \mathbf{A}_D}{\partial \rho_{ij}^{\text{MI}}} (i = 2, 3, \dots, m)$ is given as

$$\frac{\partial \mathbf{A}_D}{\partial \rho_j^{\text{MI}}} = \frac{1}{(\rho_i^{\text{MA}})^p - (\rho_{i+1}^{\text{MA}})^p} \left[\frac{\partial \mathbf{D}_i^{\text{H}}}{\partial \rho_j^{\text{MI}}} - \frac{\partial \mathbf{D}_{i+1}^{\text{H}}}{\partial \rho_j^{\text{MI}}} \right], \quad (i = 2, 3, \dots, m; j = 1, 2, \dots, n_c). \quad (5.31)$$

Specially, when $\hat{\rho}_e^{\text{MA}} \in [\rho_1^{\text{MA}}, \rho_2^{\text{MA}}]$, only the homogenized elasticity tensor $\mathbf{D}_1$ has relationship with the design variable ρ_j^{MI} , thus terms $\frac{\partial \mathbf{A}_D}{\partial \rho_{ij}^{\text{MI}}}$ and $\frac{\partial \mathbf{B}_D}{\partial \rho_{ij}^{\text{MI}}}$ are calculated by the following equations as

$$\frac{\partial \mathbf{A}_D}{\partial \rho_j^{\text{MI}}} = -\frac{1}{(\rho_1^{\text{MA}})^p - (\rho_2^{\text{MA}})^p} \frac{\partial \mathbf{D}_1^{\text{H}}}{\partial \rho_j^{\text{MI}}}, \quad (j = 1, 2, \dots, n_c). \quad (5.32a)$$

$$\frac{\partial \mathbf{B}_D}{\partial \rho_j^{\text{MI}}} = -\frac{\partial \mathbf{A}_D}{\partial \rho_j^{\text{MI}}} (\rho_1^{\text{MA}})^p, \quad (j = 1, 2, \dots, n_c). \quad (5.32b)$$

Using the adjoint variable method, the calculation of the partial differential $\frac{\partial \mathbf{D}_i^{\text{H}}}{\partial \rho_{ij}^{\text{MI}}}$ can be expressed as

$$\frac{\partial \mathbf{D}_i^{\text{H}}}{\partial \rho_{ij}^{\text{MI}}} = \frac{1}{|\mathbf{Y}|} \sum_{j=1}^{n^{\text{MI}}} \int_{\mathbf{Y}_j} (\boldsymbol{\varepsilon}^0 - \boldsymbol{\varepsilon}^* (\boldsymbol{\chi}_q))^{\text{T}} \frac{\partial \mathbf{D}_{ij}^{\text{MI}}}{\partial \rho_{ij}^{\text{MI}}} (\boldsymbol{\varepsilon}^0 - \boldsymbol{\varepsilon}^* (\boldsymbol{\chi}_q)) \, \text{d}\mathbf{y}, \quad (i = 1, 2, \dots, m), \quad (5.33)$$

where the derivative of $\mathbf{D}_{ij}^{\text{MI}}$ can be easily obtained as

$$\frac{\partial \mathbf{D}_{ij}^{\text{MI}}}{\partial \rho_{ij}^{\text{MI}}} = p \cdot (\rho_{ij}^{\text{MI}})^{p-1} \cdot (E_s^{\text{MI}} - E_0^{\text{MI}}) \cdot \mathbf{D}_0^{\text{MI}}, \quad (i = 1, 2, \dots, m; j = 1, 2, \dots, n^{\text{MI}}). \quad (5.34)$$

5.4 Numerical examples

In this section, the effectiveness of the proposed concurrent multiscale topology optimization method to design coated structures infilled with multiple self-connected microstructures is examined through several 2D benchmark design problems. Unless otherwise specified, unit cells of microstructures in the macrostructure are a square of size $1\text{mm} \times 1\text{mm}$ in all examples and design domains for multiple microstructures are all discretized into 100×100 four-node quadrilateral elements. The penalization parameter is set as $p = 4$. Because only one kind of base material is selected for structures at two scales, the material properties are given as $E_s^{\text{MA}} = E_s^{\text{MI}} = 1$ and $v_0^{\text{MA}} = v_0^{\text{MI}} = 0.3$. For projections in the proposed TO approach, the initial values of β_{PP} , β_{SP} , β_{P_1} , and β_{P_2} are all defined as 1 and respectively gradually increased with their specified increments $\Delta\beta_{\text{PP}}$, $\Delta\beta_{\text{SP}}$, $\Delta\beta_{\text{P}_1}$, and $\Delta\beta_{\text{P}_2}$ to 100. Unless otherwise specified, these parameters are given as $\Delta\beta_{\text{PP}} = \Delta\beta_{\text{SP}} = 0.5$ and $\beta_{\text{P}_1} = \beta_{\text{P}_2} = 1.0$. As for the corresponding parameters for the strict projection, the initial value of η_{SP} equals ρ_1^{MA} and $\Delta\eta_{\text{SP}}$ is set as 10^{-3} . Other design parameters are set as $\eta_{\text{PP}} = \eta_{\text{P}_1} = 0.5$. In addition, all the numerical examples are obtained by running codes written in FreeFEM++ language (Hecht, 2012). The optimization process reaches convergence if one of the following conditions is satisfied: (1) the relative change of two successive objective function values is smaller than 10^{-4} with the iteration number greater than a given value $I_{\min}$; (2) the iteration reaches the maximum allowed step $I_{\max}$. Specifically, the introduction of $I_{\min}$ can ensure the corresponding design parameters have their maximum values for a much clearer material distribution.

5.4.1 Cantilever beam design problem

In this numerical example, a cantilever beam clamped at its left edge is firstly selected to conduct the two-scale concurrent design, whose geometrical dimensions and boundary condition are presented in Fig. 5.8. Three self-connected lattice microstructures are considered and the domain extension approach (Clausen and Andreassen, 2017) is applied. The minimum and the maximum iteration numbers are set as $I_{\min} = 200$ and $I_{\max} = 300$, respectively.

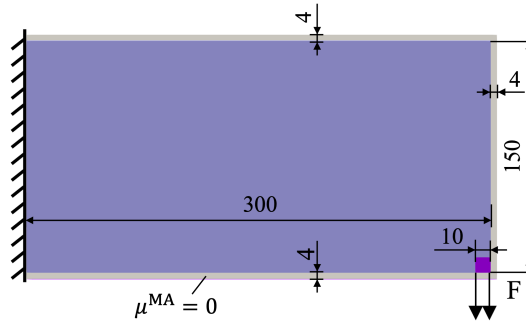


FIGURE 5.8: The structural setup for the cantilever beam design problem.

Considering different volume fractions

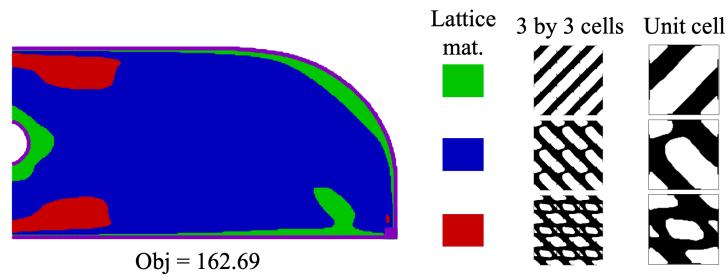
To begin with, the effect of considering different volume fractions for multiple microstructures is considered. The maximum macroscale volume fraction is defined as $f^{\text{MA}} = 50\%$ and three cases of microstructural volume fractions are considered, i.e., (a) Case 1: $f_1^{\text{MI}} = 40\%$, $f_2^{\text{MI}} = 50\%$, $f_3^{\text{MI}} = 60\%$; (b) Case 2: $f_1^{\text{MI}} = 30\%$, $f_2^{\text{MI}} = 50\%$, $f_3^{\text{MI}} = 70\%$; (c) Case 3: $f_1^{\text{MI}} = 20\%$, $f_2^{\text{MI}} = 50\%$, $f_3^{\text{MI}} = 80\%$. The thickness of the outer coating is $\omega = 3$ and the designable connective region of microstructures contains two layers of microscale elements, i.e., $T_c = 2$. The smoothing filter radii are set as $R_{S_1} = 10$ and $R_{S_2} = 8$, respectively.

The optimization processes terminated with the final static compliance value as $c=162.69$, $c=146.59$, and $c=100.42$, respectively. Fig. 5.9 presents the optimization results at two scales. As can be seen, optimized macrostructural configurations of the cantilever beam show certain similarities. However, Fig. 5.9c presents the result which has much more lattice material Mat. 3 than the ones shown in Fig. 5.9a and different layout of lattice Mat. 2 exists. These two phenomena can be attributed for a lower static compliance value that the structure in Fig. 5.9c has. At the microscale, microstructures under different volume constraints obtain varied topologies and present different directions of material distribution. Generally, the same lattice material has similar microstructural configurations, however, it can also be observed that topologies of the lattice material Mat. 3 show great difference when varied volume fractions are applied. With the variable linking over the connective region, Fig. 5.10 presents the connectivity between optimized microstructures, in which the lattice microstructural configurations are well connected in different directions. Besides, the material within the designable connective region has their unique distribution among the considered three cases. It reflects that considering different microstructural volume fractions also has certain influence on the material layout within the designable connective region.

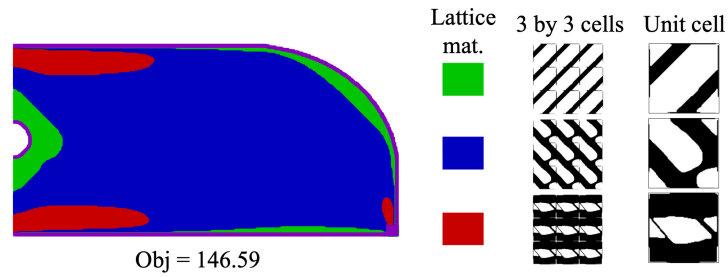
Through this example, it can be concluded that a larger difference among given microstructural volume fractions can lead to a better optimized structural performance using the proposed concurrent multiscale TO method, which is mainly attributed to the significant difference on homogenized elasticity tensors. In addition, microstructural volume constraints can change the structural topologies at the microscale but the macrostructural results are almost the same for the considered cantilever beam.

Effects of the coating thickness

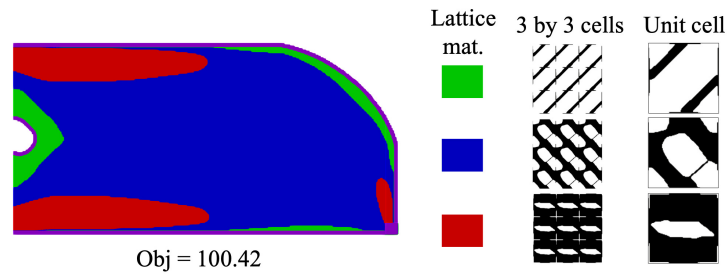
In this subsection, the effects of the coating thickness on optimization results of the coated cantilever beam infilled with three lattice microstructures are investigated. The macroscale volume fraction is defined as $f^{\text{MA}} = 50\%$ and corresponding microscale volume fractions for lattice infilling materials are set as $f_1^{\text{MI}} = 25\%$, $f_2^{\text{MI}} = 50\%$, and $f_3^{\text{MI}} = 75\%$, respectively. The thickness of the designable connective region for the connectivity issue of microstructures is given as $T_c = 3$. In



(A)



(B)



(C)

FIGURE 5.9: Optimization results at two scales of the cantilever beam considering different volume fractions: (a) Case 1, (b) Case 2, and (c) Case 3.

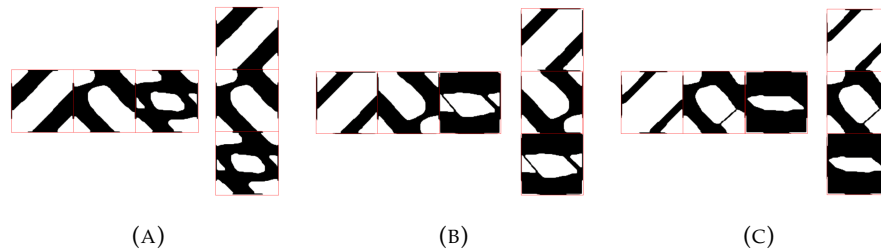


FIGURE 5.10: Connectivity of optimized microstructures for the cantilever beam considering different volume fractions: (a) Case 1, (b) Case 2, and (c) Case 3.

this numerical example, we consider three different coating thicknesses, i.e., $\omega = 3$, $\omega = 4$, and $\omega = 5$.

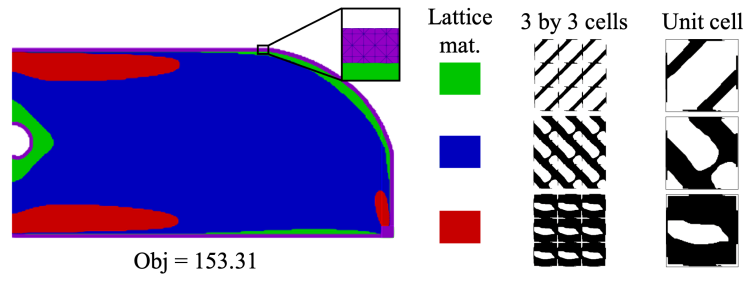
Fig. 5.11 shows the corresponding optimized macrostructures and microstructures, with the static compliance values as $c = 153.31$, $c = 133.45$, and $c = 124.86$. Reasonably, with a thicker outer coating, optimized coated structures can have a higher structural stiffness with a lower static compliance value. As those zoomed-in sub-figures presented in Fig. 5.11, the uniform thickness of the outer coating is well maintained using the proposed approach. As for the structural topologies, the variation of the coating thickness leads to highly similar structural topologies at both the macroscale and the microscale. Similar to the previous example, the lattice material Mat.2 still plays as the main role to transfer the loads from the loaded boundary to the fixed clamped ends. However, we can find that a thicker coating leads to much more material resource consumption on the coating, which on the contrary reduces the amount of material allocated to microstructures. It clearly reflects on the area of the material block for the lattice material Mat.3 within the substrate, where the macrostructure with the largest coating thickness has less Mat.3 area. Besides, there is no lattice Mat.3 exists around the loading boundary as presented in Fig. 5.11c. Optimized microstructures among three cases have the same structural topologies, which proves the coating thickness has limited effect on the microstructural configurations. The great connectivity between optimized microstructures can also be observed from Fig. 5.12. With the same material distribution over connective regions, all microstructures are well connected in different directions, proving the effectiveness of the DCR method.

5.4.2 Clamped ends beam design problem

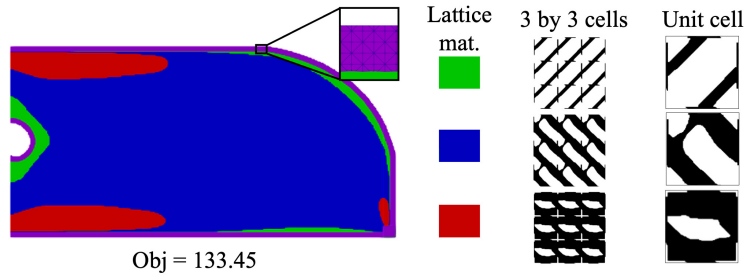
Next, a clamped ends beam is selected to further study the efficiency of the proposed multiscale TO approach. The geometrical dimensions and its boundary condition are illustrated in Fig. 5.13. A square non-design domain is modeled at the central area to apply the considered vertical load. The coating thickness is set as $\omega = 4$. With this clamped ends beam, effects of the initial microstructural guess and the thickness of the connective region on optimization results are studied.

Influence of different initial microstructural designs

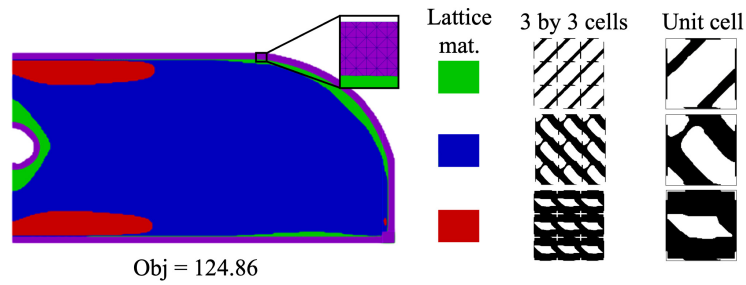
As shown in Fig. 5.14, two types of initial microstructural guess for the clamped ends beam design problem are considered. The geometrical parameters of these unit cells are depicted with dark arrows and density values are labeled with green arrows. Considering two infilling microstructures, the volume fractions at two scales are set as $f^{\text{MA}} = 50\%$, $f_1^{\text{MI}} = 50\%$, and $f_2^{\text{MI}} = 80\%$, respectively. Two layers of elements on the microstructural mesh are contained within the designable connective mesh as $T_c = 2$. Two types of microstructures are considered as the infilling materials in this numerical example.



(A)



(B)



(C)

FIGURE 5.11: Optimization results at two scales of the cantilever beam with varied coating thickness: (a) $\omega = 3$, (b) $\omega = 4$, and (c) $\omega = 5$.

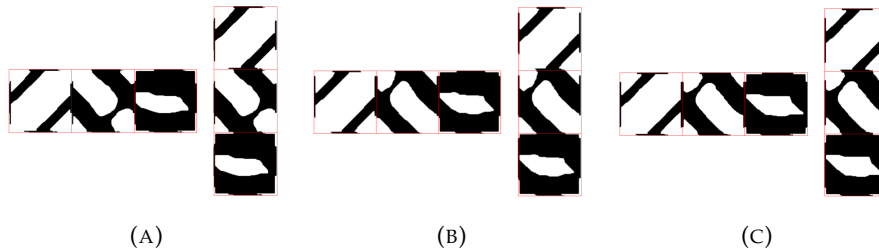


FIGURE 5.12: Connectivity of optimized microstructures for the cantilever beam with varied coating thickness: (a) $\omega = 3$, (b) $\omega = 4$, and (c) $\omega = 5$.

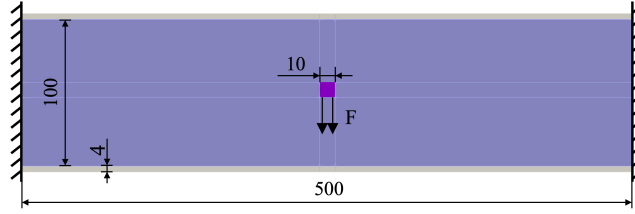


FIGURE 5.13: The structural setup for the clamped ends beam design problem.

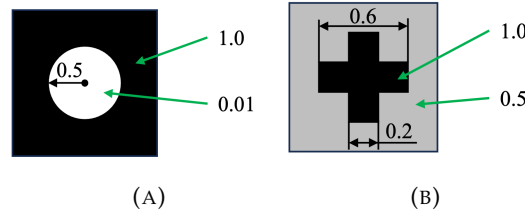


FIGURE 5.14: Two different initial microstructural guesses: (a) Initial microstructural guess No.1 and (b) Initial microstructural guess No.2.

Using the initial microstructure as shown in Fig. 5.14a and Fig. 5.14b, the optimized clamped ends beams using the proposed method with their lattice infilling microstructures are presented in Fig. 5.15 and Fig. 5.16, respectively. Generally, topologies of the macrostructure are almost the same in these two cases. With a higher stiffness, the lattice material Mat. 2 mainly distribute around the four corner of the macrostructure and form a "fallen-H" shape at the central area to better resist the external load. Due to the introduction of the volume constraint, the lattice material Mat.1 with lower allowed volume fraction still plays the main role for the structural construction. In addition, the uniform thickness of the outer coating still greatly preserved in optimized results. At the microscale, it can be clearly observed from Fig. 5.15a and Fig. 5.16a that significantly varied microstructural configurations are obtained. As shown in Fig. 5.16a, several inclined bars exist in the unit cell for the lattice material Mat.1 but the topology of the Mat.1 as shown in Fig. 5.15a has no such material layout pattern. Nevertheless, the periodic distribution of the lattice Mat.1 is similar with different initial microstructural guesses. For the lattice material Mat.2, distinct topologies are also generated, showing certain dependency on their initial guesses. Through this test, conclusions can be made that the initial microstructural guess has pretty strong influence on the optimized microstructural material layout but limited effect exist on the macrostructural configuration.

With different initial microstructures, optimization processes respectively take 212 and 217 iteration steps to converge with the final static compliance as $c = 739.11$ and $c = 746.26$, as shown in Fig. 5.15b and Fig. 5.16b. Despite several ups and downs during the early optimization process because of the searching on the external coating and layout of multiple infilling lattice materials, iteration histories of the multiscale design of the clamped ends beam are pretty stable with both the objective function and considered volume constraints smoothly converge. This iteration

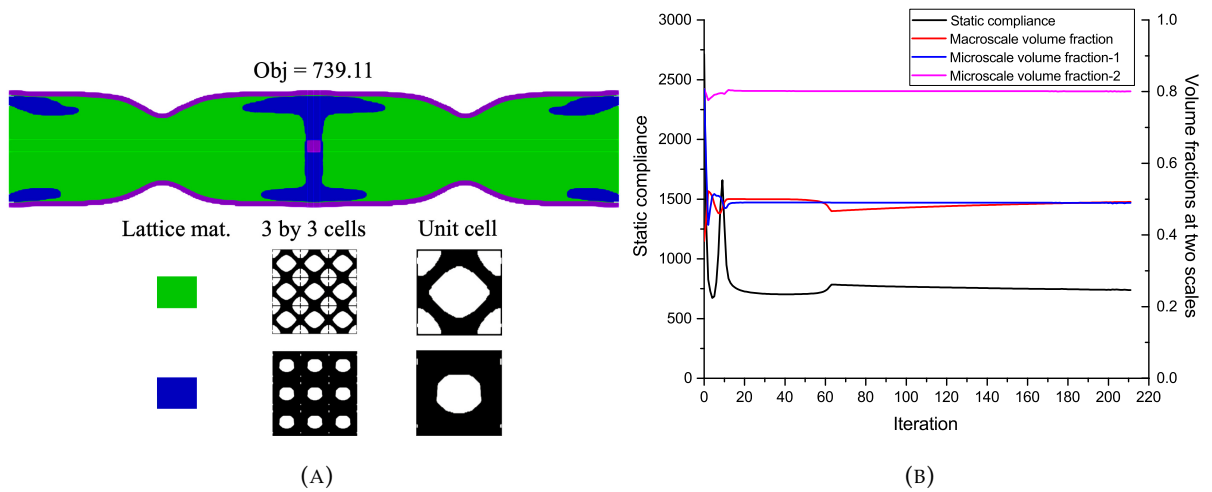


FIGURE 5.15: The results of the clamped ends beam with the initial microstructural guess No.1: (a) optimized structures at two scales and (b) iteration history.

performance reveals that the proposed TO method greatly inherit the advantage of the original ordered SIMP method. Besides, it also proves that the effectiveness of using a stable growth of design parameters in the proposed filtering procedure.

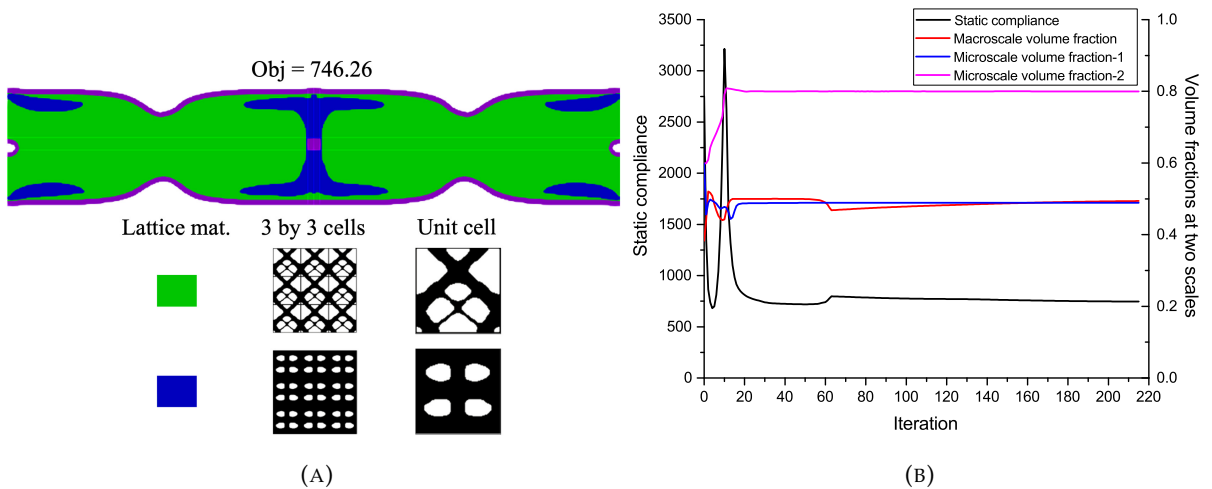


FIGURE 5.16: The results of the clamped ends beam with the initial microstructural guess No.2: (a) optimized structures at two scales and (b) iteration history.

The connectivity of optimized microstructures is given in Fig. 5.17. As can be seen, the material distribution within the designable connective region still ensures these optimized microstructures have great connectivity, both in the horizontal and the vertical directions.

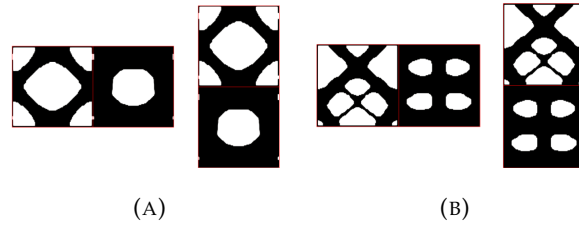


FIGURE 5.17: Connectivity of optimized microstructures for the clamped ends beam considering different initial microstructures: (a) using the initial microstructural guess No.1 (b) using the initial microstructural guess No.2.

Effects of the connective region thickness

In this numerical example, we examine how can the connective region thickness affect optimized designs at two scales using the proposed approach. Three types of microstructures are considered as the lattice infilling materials for the clamped ends beam, with their maximum volume fractions set as $f_1^{\text{MI}} = 30\%$, $f_2^{\text{MI}} = 50\%$, and $f_3^{\text{MI}} = 80\%$, respectively. The macroscale volume fraction is given as $f^{\text{MA}} = 50\%$. For the smoothing filtering operation, radii are set as $R_{S_1} = 6$ and $R_{S_2} = 6$, respectively.

With varied connective region thicknesses, optimized macrostructures and their corresponding microstructural configurations are presented in Fig. 5.18, with the static compliance values as $c = 701.61$, $c = 715.10$, and $c = 728.37$. As can be seen, various lattice microstructures share similar distribution at the macroscale among three cases and the lattice material Mat.2 plays as the main material to constitute the macrostructure, mainly due to its relative balance on the stiffness contribution and material consumption. With the stiffest homogenized elasticity tensor, the obtained layout of the lattice material Mat.3 can better resist the external load and transfer it to the fixed boundaries. Moreover, we can observe that some isolated material blocks for the Mat.3 exist at the central area of the beam (as shown in Fig. 5.18c) when a larger connective region thickness is applied, reflecting the interaction of structures at two scales during the optimization process. At the microscale, even though some limited differences present over their predefined connective regions, microstructures marked by the same color share the same structural topologies. Fig. 5.19 shows the connectivity of optimized microstructures, in which the connectivity is well ensured in both the horizontal and vertical directions. It should be noted that the designable connective regions of different connective region thickness cases are almost all filled with solid base material. Explanation can be given for this phenomenon as such material layout offers the lattice material Mat.3 a better homogenized material properties and the variable linking technique we introduced. In general, we can conclude that the variation of the connective region thickness has limited effect on obtained optimization results. However, with a larger connective region thickness, the design freedom of the problem is reduced, leading to a higher static compliance value.

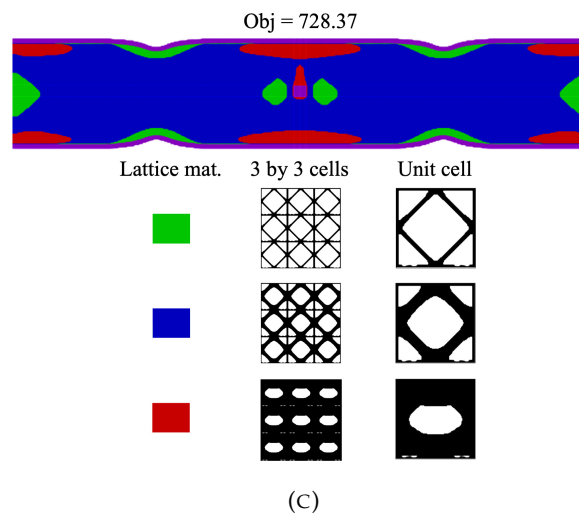
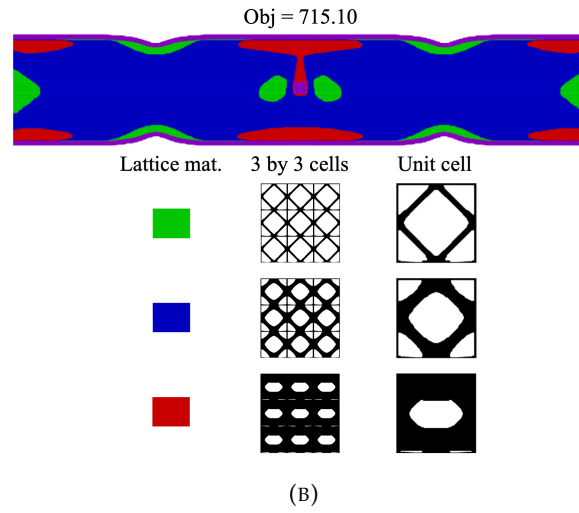
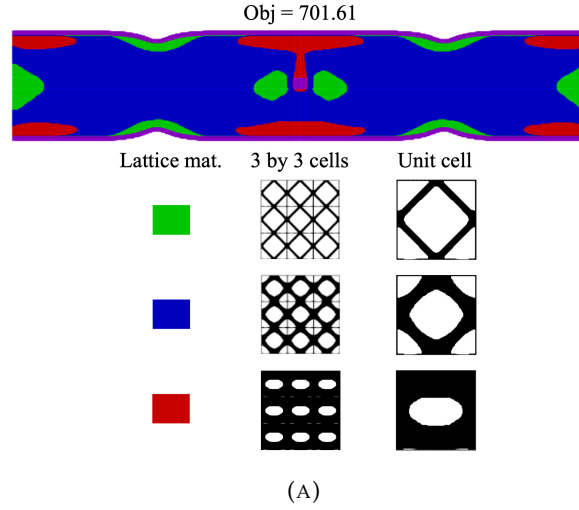


FIGURE 5.18: Optimization results at two scales of the clamped ends beam considering different connective region thicknesses: (a) $T_c = 2$, (b) $T_c = 3$, and (c) $T_c = 4$.

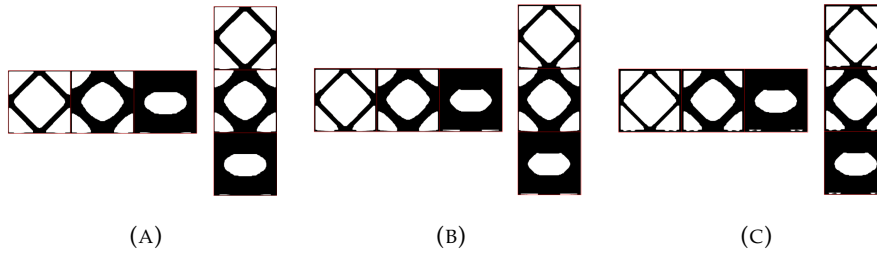


FIGURE 5.19: Connectivity of optimized microstructures for the clamped ends beam considering different connective region thicknesses: (a) $T_c = 2$, (b) $T_c = 3$, and (c) $T_c = 4$.

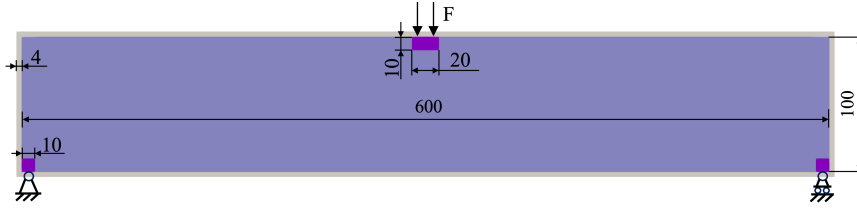


FIGURE 5.20: The structural setup for the MBB beam design problem.

5.4.3 MBB beam design problem

As the next example, a typical MBB (Messerschmitt Bolkow Blohm) beam is introduced to study the influence of considering different number of lattice microstructures. The geometrical parameters of the macroscale domain are illustrated in Fig. 5.20. As for the mesh size, the macrostructure is discretized into 304×54 finite number of elements and unit cells of considered microstructures are all discretized in 80×80 elements, respectively. With the coating thickness defined as $T_c = 2$, three infilling cases are considered in this MBB beam design problem, i.e., (a) single infilling microstructure, (b) two infilling microstructures, and (c) three infilling microstructures. Specially, in order to make a reasonable comparison and eliminate the effect of microstructural volume fractions, the maximum allowed macroscale volume fraction is set as $f^{\text{MA}} = 50\%$ and the microstructural volume fractions are defined as (a) $f_1^{\text{MI}} = 60\%$, (b) $f_1^{\text{MI}} = 40\%$, $f_2^{\text{MI}} = 80\%$, and $f_1^{\text{MI}} = 40\%$, $f_2^{\text{MI}} = 60\%$, and $f_3^{\text{MI}} = 80\%$, respectively.

Corresponding optimized macrostructures and their lattice microstructural configurations are presented in Fig. 5.21. Obviously, varied topologies of macrostructures can be obtained when different number of infilling microstructures is considered. Different from other two cases, the MBB beam infilled with a single microstructure has a void domain in its central area, as shown in Fig. 5.21a. For the two-microstructure and three-microstructure cases, there is no internal holes generated and the lattice material Mat. 1 is the main material for the structural constructions. With higher allowed volume fractions, a horizontal distribution of the lattice materials Mat. 2 and Mat. 3 concentrated at the upper and lower parts of the structure can be seen in Fig. 5.21c, which can effectively transfer the loads from top-loaded boundary to fixed boundaries at the bottom. Similar

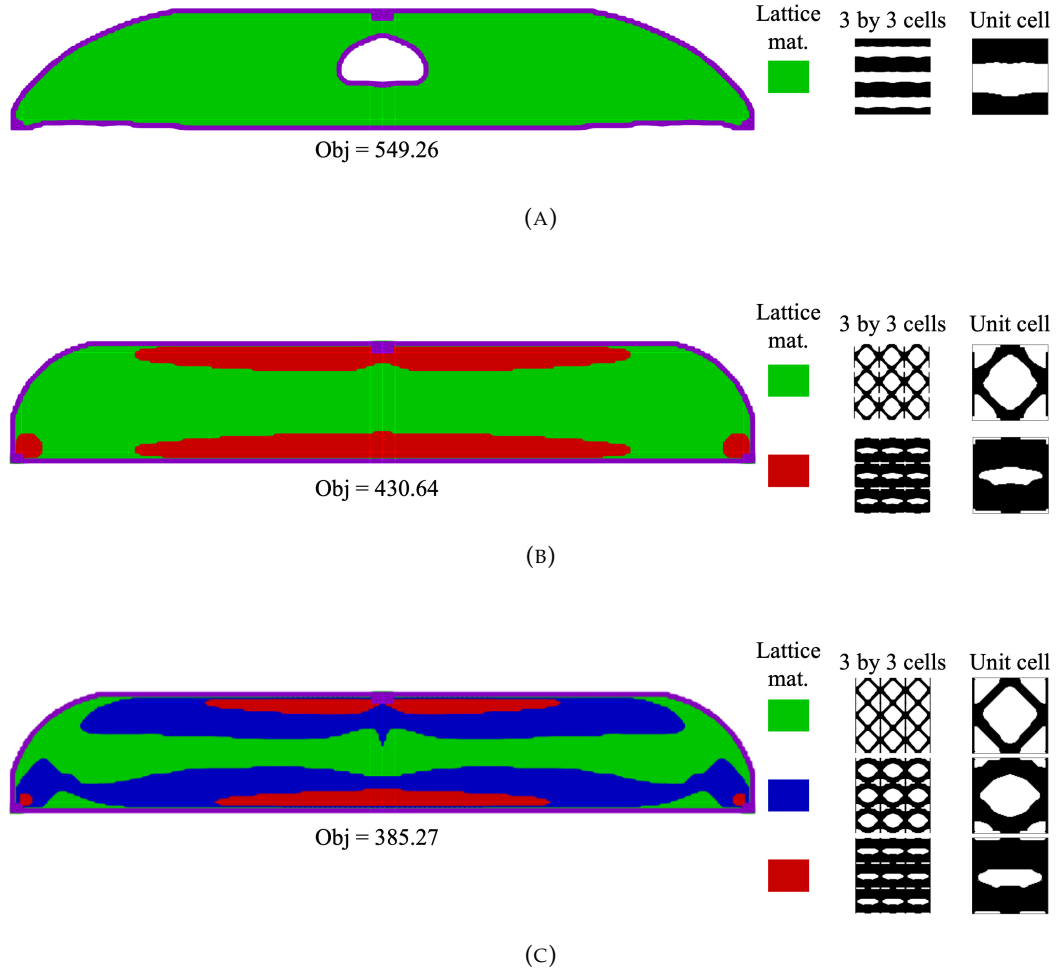


FIGURE 5.21: Optimization results at two scales of the MBB beam considering different number of microstructures: (a) one microstructure, (b) two microstructures, and (c) three microstructures.

phenomenon can also be observed in the two-infilling-material case, as presented in Fig. 5.21b. With different volume fractions applied, varied microstructural topologies are obtained. When a single lattice material is optimized for the MBB beam, the base material exhibits a horizontal layout within the unit cell, as shown in Fig. 5.21a. The microstructural configurations having the same maximum volume fractions are similar with each other in the Cases (b) and (c). Sharing the same material distribution within their designable connective regions, connectivity between optimized microstructures are still well-preserved in both the horizontal and vertical directions, as shown in Fig. 5.22.

Under the same material consumption at the macroscale, static compliance values of structures presented in Fig. 5.21 are $c = 549.26$, $c = 430.64$, and $c = 385.27$, respectively. With reasonable microstructural volume fractions, it can be reported through this example that coated structures considering more kinds of microstructures can lead to better structural performance to a large extent.

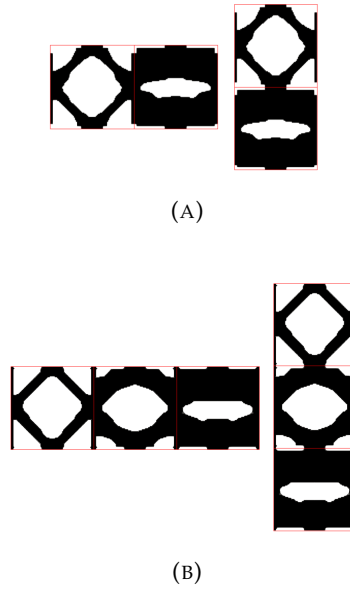


FIGURE 5.22: Connectivity of optimized microstructures for the MBB beam: (a) two microstructures and (b) three microstructures.

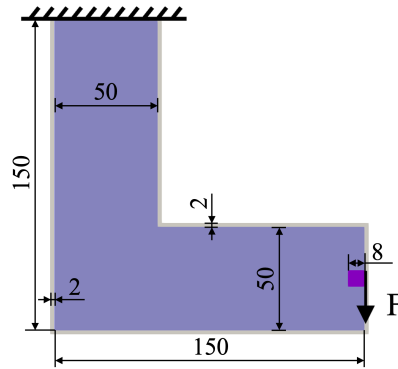


FIGURE 5.23: The structural setup for the L-shaped beam design problem.

5.4.4 L-shaped beam design problem

A L-shaped beam as shown in Fig. 5.23 under a vertical load is selected to further test the effectiveness of the proposed concurrent multiscale TO framework. In this example, the necessity of considering microstructural connectivity is tested and a comparison on the calculation accuracy is performed.

Comparison between designs w/o considering the connectivity

For comparison, Fig. 5.24 shows the optimized coated L-shaped beam with and without considering the connectivity between microstructures, under the same macroscale constraint as $f^{\text{MA}} = 40\%$. Obviously, optimized macrostructural configurations share the same topology and have

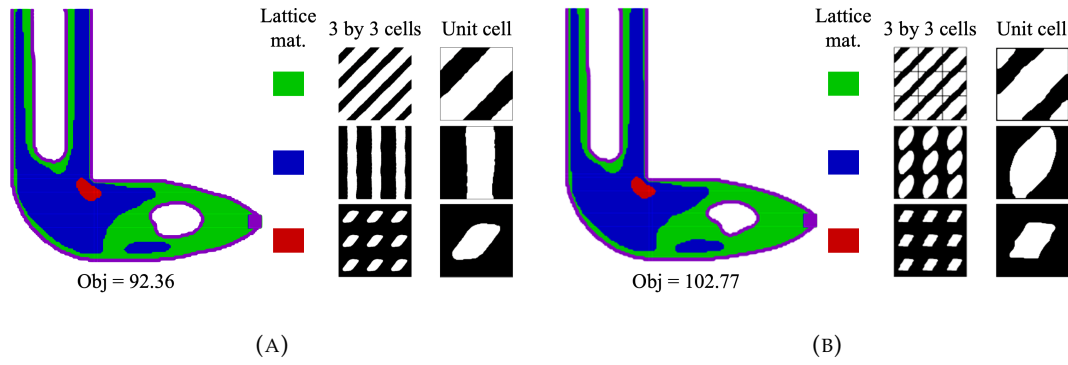


FIGURE 5.24: Optimization results at two scales of the L-shaped beam: (a) without considering the microstructural connectivity and (b) using the introduced DCR method.

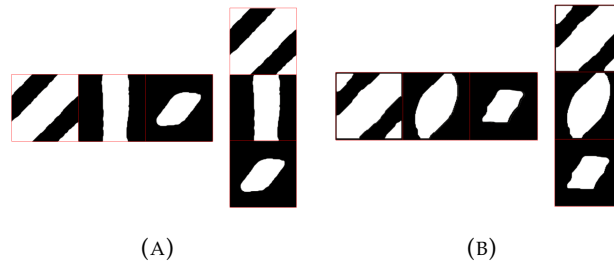


FIGURE 5.25: Connectivity of optimized microstructures for the L-shaped beam: (a) without considering the microstructural connectivity and (b) using the introduced DCR method.

resembling layout of the lattice material blocks. To resist the deformation caused by the external force, the lattice material Mat.2 mainly distribute at the left part of the beam and directly connected to the top fixed boundary. On the contrary, the lattice microstructural material Mat.1 works as the main infilling for the right part of the L-shaped beam. In both cases, it can be found that the stiffest lattice material Mat.3 reasonably allocate around the turning corner of the beam, where the stress is most concentrated and thus the stiffness of the structure can be effectively improved. With and without considering the connectivity issue, topologies of optimized microstructures have certain similarities. However, the unit cell of the material Mat.1 contains particular material around its edges, which cannot be seen in the case without the connectivity consideration (Fig. 5.25a), due to the variable linking used in the DCR method. Additionally, for the lattice material Mat.2 presented in Fig. 5.25a, the base material is formed in the vertical direction, similar to its distribution at the macroscale. But as shown in Fig. 5.25b, the base material in Mat.2 has inclined layout because of the existence of material within the connective region to better contribute homogenized elasticity tensor. As for the lattice material Mat.3, no big structural difference exist between the optimized results.

From Fig. 5.25, we can clearly see that the microstructures optimized with no connectivity considered have poor structural connectivity, especially for the lattice materials Mat.1 and Mat.2 in the vertical direction. Definitely, such optimization results cannot be successfully manufactured using the AM technique. As shown in Fig. 5.25b, the microstructural configurations optimized using the proposed method achieve self-connectivity in both directions. With this numerical example, the necessity of taking microstructural connectivity into consideration and the effectiveness of the DCR method are both proved. Although the introduction of the DCR method will reduce the design freedom and generate a coated structure with comparatively higher static compliance value (about 10% higher in Fig. 5.24), the final optimized macrostructure with its multiple microstructures is totally manufacturable.

5.4.5 Performance verification

In order to verify the calculation accuracy of the structural performance, a single-scale model of the optimized L-shaped beam is constructed, based on the optimization results presented in Fig. 5.24b. Using the commercial software COMSOL Multiphysics (COMSOL Multiphysics, n.d.), the optimized macrostructure is firstly constructed and the microstructural topologies are modeled within the substrate of the coated structure. Next, with the repetition of microstructures covering all the specific material blocks, a boolean operation is performed to generate the single-scale coated structure by mixing the structures at two scales, yielding a geometrical model as presented in Fig. 5.26. Thanks to the consideration of the microstructural connectivity, the geometrical model of microstructures can be successfully created, as shown in those zoomed-in figures in Fig. 5.26. It should be point out that there is no need to separate the domain of the coating and microstructures from the geometrical model, because only one base material is used for structures at two scales in the developed method. Eventually, a finite element model using the body-fitted mesh is created for the further numerical analysis, as shown in Fig. 5.27, which composed of more than 3.2 million triangular elements with geometrical details well described.

The calculated static compliance value of the L-shaped beam as presented in Fig. 5.27 is 106.60, which is about 4 % larger than the one obtained using the proposed method. Considering the large difference on the number of elements between the two models, it can be concluded that the proposed multiscale TO method for the design of coated structures has pretty great calculation accuracy.

5.4.6 3-load short beam design problem

Finally, a short beam under three loads applied on its lower boundaries is selected to check the manufacturability of the results obtained using the developed approach. The dimensions and

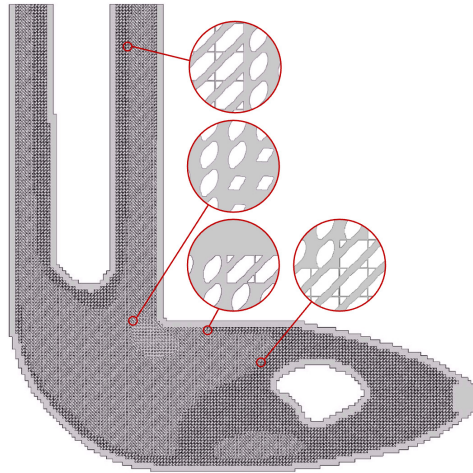


FIGURE 5.26: The geometrical model of the optimized L-shaped beam infilled with self-connected microstructures.

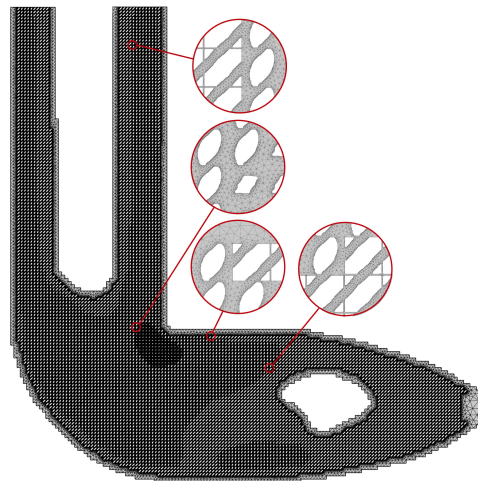


FIGURE 5.27: The finite element model of the optimized L-shaped beam infilled with self-connected microstructures.

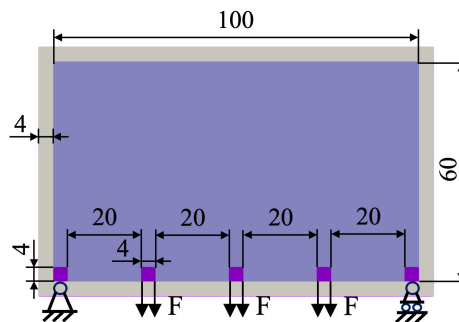


FIGURE 5.28: The structural setup for the 3-load short beam design problem.

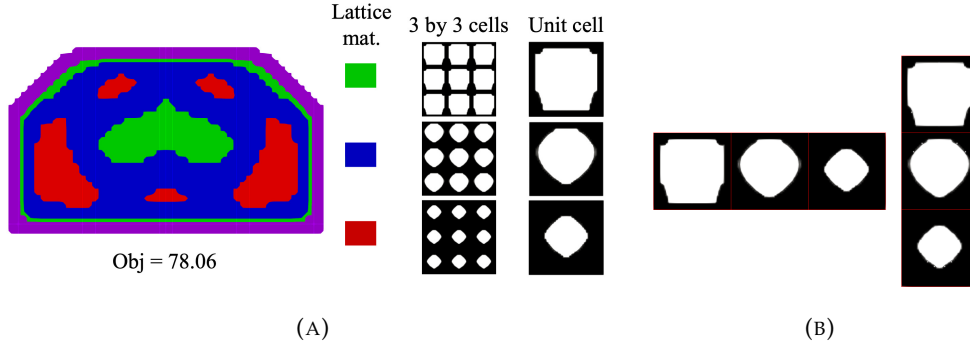


FIGURE 5.29: Optimization results at two scales of the L-shaped beam: (a) without considering the microstructural connectivity and (b) using the introduced DCR method.

boundary conditions of the beam are illustrated in Fig. 5.28. To meet the manufacturing requirements, comparatively coarser meshes are generated in this example, with the macroscale domain discretized into 54×34 elements and 40×40 microscale elements for all microstructures, respectively. Three types of lattice microstructural materials are considered, with varied maximum volume fractions applied, i.e., $f_1^{\text{MI}} = 40\%$, $f_2^{\text{MI}} = 60\%$, and $f_3^{\text{MI}} = 80\%$. The upper limit of the macroscale volume fraction is set as $f^{\text{MA}} = 50\%$ and 4 layers of microscale elements are counted into the designable domain of microstructures, i.e., $T_c = 4$.

The optimization results at two scales are presented in Fig. 5.29a. At the macroscale, the microstructural material Mat.2 contributes the main of the lattice infilling, with several isolated islands composed of the lattice material Mat. 3. The layout of the microstructure with the smallest allowed volume fraction mainly concentrated at the central area of the structure. With clear distribution of material blocks at the macroscale, the optimized microstructures show great connectivity with each other, as shown in Fig. 5.29b. With three loads applied, the final static compliance value of the obtained result is $c = 78.06$. Based on the optimization results at two scales as shown in Fig. 5.29, a single-scale model is constructed and manufactured using the AM technique with self-connected infilling microstructures successfully printed, as presented in Fig. 5.30. Through this short beam example, the manufacturability of coated structures infilled with multiple self-connected microstructures designed using the developed approach is well verified.

5.5 Summary

In the present study, a novel density-based multiscale TO method is proposed to concurrently optimize macrostructural configurations and multiple self-connected lattice infilling microstructures of coated structures. Based on the ordered SIMP method, the spatial distribution of different infilling material blocks over the macrostructure is firstly described by using a piece-wise projection towards the macroscale design variable field. After implementing the novel strict projection, the

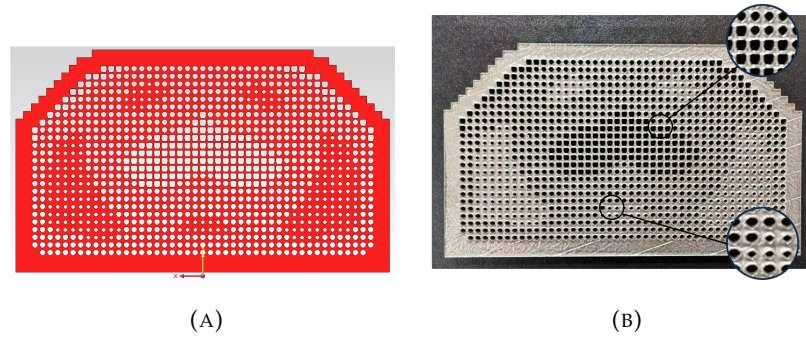


FIGURE 5.30: The single-scale 3-load short beam: (a) .STL file and (b) Structure manufactured via the AM technique.

classical two-step filtering operation is applied to identify the external coating and the infilling region of coated structures. Then, the layout of material blocks for lattice microstructures is gradually formed and described by mixing the previous piece-wisely projected field with the substrate identification field during the optimization. To fully consider the interaction between structural evolution at two scales, topologies of multiple microstructures are simultaneously designed with their macroscale distribution, and the connectivity of them is dealt with by the DCR method to achieve self-connected property.

Using the proposed method, the actual material consumption of a coated structure can be controlled by a single macroscale volume constraint due to the same base material applied for the structures at two scales. Besides, the corresponding example reveals that a larger difference on the considered microstructural volume fractions assigned towards different lattice materials results in a better structural performance. From the view of the authors, this is because of a better optimum searching ability induced by the clearer distinction on homogenized material properties under the ordered SIMP framework. The effects of other important factors on optimization results are also investigated, such as coating thickness, initial microstructural guess, connective region thickness, and the number of considered microstructures. According to corresponding numerical results, it is found that the proposed approach can successfully handle different coating thicknesses and stiffer coated structures can be obtained with a thicker outer coating. Besides, the initial microstructural guess has a significant influence on optimized topologies of lattice microstructures, but no obvious difference can be reported on the macrostructural configurations. When different connective region thicknesses are applied, similar macrostructures and microstructures are obtained, displaying the predefined connective thickness may have little effect on optimized topologies. However, the design freedom of the optimization problem will be reduced with a large value of the connective region thickness and yields a higher static compliance. Also, considering more kinds of lattice microstructural materials with rational volume fraction setting has the potential to further improve the structural performance of optimized coated structures. The necessity of considering the microstructural connectivity in the multiscale design problems is well verified in the L-shaped

beam example, as well as the calculation accuracy of the developed approach. And all the numerical examples using the DCR method demonstrate great geometrical connectivity at the microscale, and thus the effectiveness is well verified.

Chapter 6

Topology optimization of coated structures with non-uniform coating thickness[†]

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6.1 Introduction

Typically composed of an external coating and a porous infill, coated structures are commonly found in the natural world, examples of which include bird beaks and human bones (as shown in Fig. 6.1). Functionally, the external coating of coated structures provides protection to the inner substrate, while the substrate forms the main body of the structure with the maintenance of its

[†]The work in this chapter has been submitted to *Structural and Multidisciplinary Optimization* (Springer).

strength. Coated structures exhibit several outstanding properties, such as a high stiffness-to-weight ratio and excellent buckling resistance (Wu, Clausen, and Sigmund, 2017; Clausen, Aage, and Sigmund, 2016). Additionally, Liu et al. (Liu, Lai, Lu, Zhou, and Lin, 2023) found that coated structures with porous infilling demonstrate superior energy absorption capabilities.

Topology optimization (TO) is one of the most powerful design tools in the field of structural optimization. Compared to its competitors, i.e., size optimization and shape optimization, TO excels in its ability of allocating the material distribution in the optimal form with nucleation of holes to achieve the best performance while adhering to certain constraints. Since the pioneering research of Bendsøe and Kikuchi (Bendsøe and Kikuchi, 1988), TO has rapidly evolved over the past decades with many useful TO approaches being proposed, including solid isotropic material with penalization (SIMP) method (Bendsøe and Sigmund, 1999; Sigmund, 2001; Andreassen, Clausen, Schevenels, Lazarov, and Sigmund, 2011), level set (LS) method (Wei, Li, Li, and Wang, 2018; Challis, 2010; Wu, Zhu, Gao, Gao, and Liu, 2024), evolutionary structural optimization (ESO) method/bi-directional ESO (BESO) method (Xie and Steven, 1996; Xia, Xia, Huang, and Xie, 2018), method of moving morphable components/voids (MMC/MMV) method (Zhang, Song, Zhou, Du, Zhu, Sun, and Guo, 2018; Zhang, Li, Yuan, Song, and Guo, 2017; Zhang, Chen, Zhu, Zhou, Xue, Lei, and Guo, 2017), etc. Especially, due to the rapid development of additive manufacturing (AM), the complex structures optimized via the TO technique can be effectively fabricated now, which further facilitates the advancement of TO.

Designing coated structures using TO is becoming increasingly popular within the optimization community and it has been applied in various fields, including the patient-specific biological implant design (Nickels, 2012b) and 3D meta-structure optimization for vibration mitigation (Matlack, Bauhofer, Krödel, Palermo, and Daraio, 2016). The first research on the TO of coated structures was studied by Clausen et al. (Clausen, Aage, and Sigmund, 2015), in which a classical two-step filtering process is developed for the identification of the outer coating with the calculation of a smoothed density field's spatial gradient. After that, Clausen et al. (Clausen,

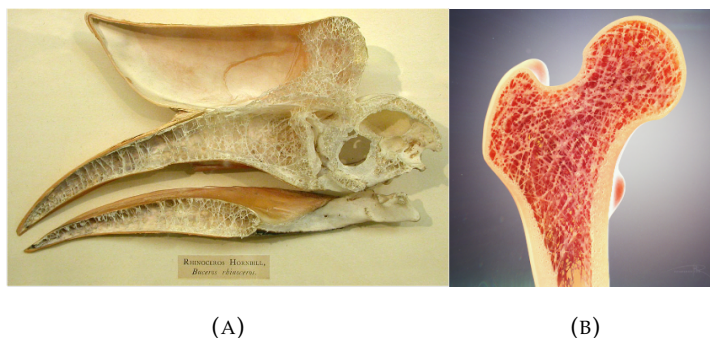


FIGURE 6.1: Coated structures in the natural world: (a) Horbill bird beak (Aage, Andreassen, Lazarov, and Sigmund, 2017) and (b) human bone (www.kashpersky.com).

Andreassen, and Sigmund, 2017) further verified the effectiveness of this two-step filtering procedure in 3D problems. Without the gradient calculation, Yoon and Yi (Yoon and Yi, 2019) developed a new density-based coating filter for identifying the coating using the original field and its modified field. Subsequently, Yi et al. (Yi, Yoon, and Peng, 2021) improved their work and distinguished the coating and the substrate using the smoothed and projected density variables. Luo et al. (Luo, Li, and Liu, 2019) proposed an erosion-based interface identification method for the design of coated structures, in which the theoretical relation between the erosion parameters and the coating thickness is derived. Groen et al. (Groen, Wu, and Sigmund, 2019) developed a novel homogenization-based TO method to design coated structures with orthotropic infill. Using a phase field-based TO approach, Xie et al. (Xie, Feng, Xia, Kim, and Li, 2024) identified the coating based on initial TO results and designed coated structures with microstructural infill. Postigo et al. (Postigo, Garaigordobil, Ansola, and Canales, 2024) introduced a SUSAN (Smallest Univalued Segment Assimilating Nucleus) algorithm into the two-step filtering procedure and proposed a new TO method to design coated structures with control of coating thickness and minimum length scale for AM. Till now, density-based TO of coated structures have been applied for various functionalities, such as natural frequency optimization (Liu, Bai, Yao, and Luan, 2022), multimaterial infills (Hu, Wang, Li, Yu, Furuta, Izui, and Nishiwaki, 2024), and stress constraints (Wang and Wu, 2024). Without any filtering or projections, LS methods exhibit natural advantages in designing coated structures for its easy maintenance of the coating thickness due to the signed distance property. The first research on TO of coated structures using the LS method was studied by Wang and Kang (Wang and Kang, 2018a), in which two LS values of a LS function are utilized to describe the coating thickness. In the research of Fu et al. (Fu, Li, Xiao, Gao, and Chu, 2019), the parametric LS function is regularized to a signed distance function using a distance regularization term and studied the coated structure using a new parametric LS method. This regularized parametric LS method was then extended to the multiscale TO coated structures (Fu, Li, Gao, and Xiao, 2019). Using the signed distance property of the velocity field-based LS method, Hu et al. (Hu, Wang, Zhang, Li, Ding, Izui, and Nishiwaki, 2022; Hu, Wang, Zhang, Li, Ishida, Sasaki, Furuta, Izui, and Nishiwaki, 2023) addressed TO of coated structures considering dynamic structural performance. Jiang et al. (Jiang, Guo, Chen, Wei, Lei, and Gu, 2019) constructed a new kind of cardinal basis function (CBF) for the LS parameterization and designed coated structures infilled with conformal mapped microstructures using a CBF-based LS method. In the research of Bai and Zuo (Bai and Zuo, 2022), multiple LS surfaces are utilized to optimize the multi-material infilling of coated structures and one LS surface with signed distance property is selected for the coating description. Some researchers also conducted the optimum design of coated structures using other TO methods, such as BESO method (Qiu, Jin, Jin, Wang, Xia, Zhu, and Shi, 2020) and adaptive geometrical components approach (Hoang, Tran, Nguyen, Hackl, and Nguyen-Xuan, 2020).

Although plenty of research on TO of coated structures have been achieved, it is important to note that almost all of these studies assume a uniform coating thickness. In other words, the external coating maintains the same thickness throughout, with a fixed value. However, coated structures in nature often display varying coating thickness. For example, as shown in Fig. 6.1b,

the coating (cortical bone area) of human bones is thicker at the base, which helps the bone better adapt to external environments and stimuli. Thus, while a uniform coating thickness can lead to good performance, it also limits the design freedom of the optimization problem and fails to fully exploit the potential of coated structures. To the best knowledge of the authors, only the research of Yang et al. (Yang, Gao, and Li, 2024) has considered the non-uniform coating during the TO process for coated structures. However, in their study, the coating thickness was determined by a displacement-related formula (larger deformations result in greater thickness) and focused on improving resistance to fatigue, corrosion, and abrasion, rather than optimizing the considered objective function. Therefore, the corresponding research is lack of study and this motivates us to explore non-uniform coating thickness in the design of coated structures to achieve improved structural performance.

Generating smooth structural boundaries in TO results is highly attractive for both academia and industry due to its potential for rapid conversion into CAD models, enabling faster manufacturing processes. LS methods still exhibit significant advantages towards this issue that the structural boundaries are naturally smooth due to the implicit structural representation via the LS function. In contrast, density-based methods often lead to results with unsmooth structural boundaries because they rely on discretized meshes. Additionally, the continuous variation in density at the boundaries of those results also bring difficulties to the CAD model construction. Compared to LS or component-based TO approaches, such as MMC and MMV methods, density methods present greater challenges in achieving smooth structural boundaries. Based on the TO of binary structures (TOBS) method, Costa Azevêdo et al. (Costa Azevêdo, Li, Ishida, Siqueira, Cortez, Nelli Silva, Nishiwaki, and Picelli, 2024) introduced a geometry trimming approach in the optimized binary density fields for smoothed edges, in which a nodal iso-surface function with a spatial nodal filter is constructed to create the body-fitted mesh. In the research of Da et al. (Da, Xia, Li, and Huang, 2018), sensitivity values were transferred from elements to nodes via a heuristic filter (Sigmund and Petersson, 1998), and a nodal sensitivity-based LS function was constructed for smooth boundary representation. Li et al. (Li, Qin, Wei, and Su, 2022) proposed a novel boundary density evolution (BDE) method which refines structural boundary elements based on the LS surface using nodal strain energy. Additionally, by applying a sensitivity threshold, Li et al. (Liu, Guo, Jiang, Li, and Huang, 2019) created a continuous function from the sensitivity information of the structure to obtain smooth structural boundaries. Even though these studies offer smooth structural representations, designing coated structures with smooth boundaries via density methods remains largely unexplored, which arises our interest to advance this area further.

This study proposes a new density-based TO method for the optimum design of coated structures. Different from previous research, the developed approach in this paper optimizes the coating with variable thickness to enhance structural performance and achieves smooth boundary representation through a post-processing optimization. Specifically, an improved PDE filter is incorporated into the classical two-step filtering process to identify the coating along the design domain boundaries, significantly simplifying the modeling process. In addition to the density field,

the filter radius field of the improved PDE filter is treated as a design variable to implicitly adjust the coating thickness through two modified density fields. After obtaining an optimized result on a fixed mesh, a post-processing optimization is performed to refine the structural topology. The coating identification field is used to construct the LS function for the identification of structural boundaries, and a body-fitted mesh is generated using the Mmg platform (Dapogny, Dobrzynski, and Frey, 2014) during post-processing. The compliance minimization problem is investigated to validate the developed approach, with sensitivities for objective functions and volume constraints derived accordingly. The advantages of considering non-uniform coating thickness in the design of coated structures are evaluated numerically, and the effectiveness of the proposed method is demonstrated through several 2D examples.

The reminder of this paper is organized as follows. Section 6.2 introduces the material modeling process of coated structures with non-uniform coating thickness. In Section 6.3, formulations for the TO problem are constructed and the techniques of the post-processing optimization for smooth structural representation are introduced. Section 6.4 derives the sensitivity analysis for different design variables and several numerical examples are demonstrated in Section 6.5. Finally, concluding remarks are provided in Section 6.6.

6.2 Material modeling of coated structures with non-uniform coating thickness

6.2.1 Problem description

Fig. 6.2 illustrates the structural configuration we aim to design in the presented paper, wherein the infilling material constitutes the primary structure and is enveloped by a solid external coating with variable thickness. Apart from the innovative non-uniform coating, the coated structure displayed has a smooth boundary presentation, which we plan to achieve through a novel density-based TO method. To validate the practicality of the developed approach, the compliance minimization problem is investigated and the formulation will optimize the structural topology with the coating thickness simultaneously for enhanced structural performance. A new two-step filtering procedure using non-homogeneous filter radius is developed to define the variable coating thickness.

Since two materials are considered in this study, two mass constraints are applied to control the material consumption for the entire structure and the non-uniform coating, separately. As mentioned before, density-based methods usually lead to optimized results with zig-zag structural boundaries, thus, a level set function is created to produce smooth boundaries, with a post-processing optimization further conducted to meet the structural mass constraints.

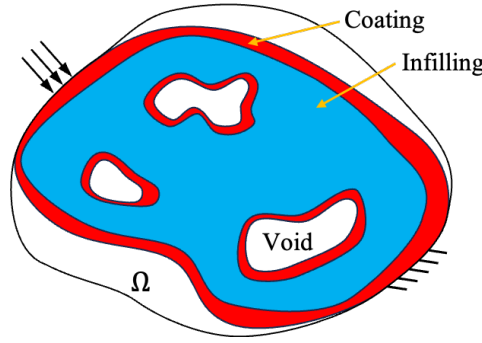


FIGURE 6.2: Schematic illustration of coated structures with non-uniform coating thickness and smooth structural boundaries

6.2.2 Design method of coated structures with non-uniform coating thickness

This subsection provides a detailed introduction to the method for optimizing coated structures with variable coating thickness. Using one density variable field, the coating is separated through two modified density fields generated by a new filtering and projection process, as shown in Fig. 6.3. Different from other research works, the filter radius field in the second PDE filtering in the developed approach is not homogeneous but selected as the other type of design variables and optimized to be non-homogeneous during TO. For clarity, the key techniques involved are presented first as follows.

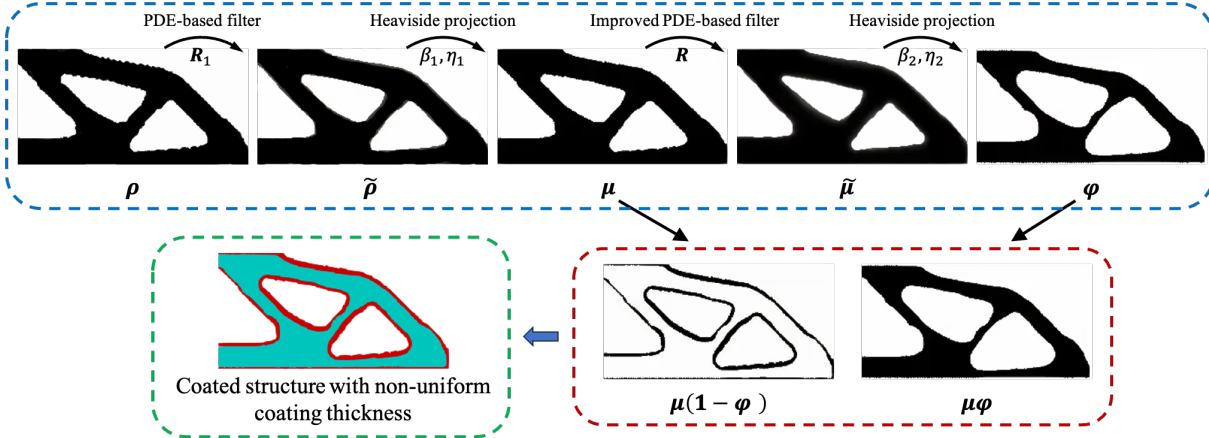


FIGURE 6.3: The new two-step filtering and projection procedure for coated structures with non-uniform coating thickness.

PDE-based filter

As shown in Fig. 6.3, the original design variable field ρ is firstly smoothed using a commonly applied PDE filter based on a Helmholtz-type partial differential equation (Lazarov and Sigmund,

2011), where the filtered density field $\tilde{\rho}$ is implicitly defined as the solution to the following formula:

$$\begin{cases} -r_1^2 \frac{d^2 \tilde{\rho}}{dx^2} + \tilde{\rho} = \rho \\ \tilde{\rho}|_{x \rightarrow -\infty} = 0, \tilde{\rho}|_{x \rightarrow \infty} = 0 \end{cases} \quad (6.1)$$

where r_1 is the length scale. Working as an isotropic filter in the developed two-step filtering process, the length scale in Eq. (6.1) is uniform and obtained from a uniform filter radius field R_1 , with the numerical relationship as

$$r_1 = \frac{R_1}{2\sqrt{3}} \quad (6.2)$$

Improved PDE-based filter

One of the differences between the two-step filtering and projection procedures used in the developed method and other approaches lies in the second PDE filtering. To simplify the modeling process of designing coated structures, Gao et al. (Gao, Yang, Zhang, and Liu, 2023) proposed an improved PDE filter to address the boundary effects in the standard PDE filter by finding a rational value of non-homogeneous Neumann boundary conditions. As a result, the coating can be successfully identified along the boundaries of the design domain and no domain extension method is needed for the finite element model construction. Therefore, instead of using the above PDE-based filter, the improved PDE-based filter is introduced to filter the modified density field μ in the proposed method for the coating identification, which can be formulated as

$$\begin{cases} -r^2 \frac{d^2 \tilde{\mu}}{dx^2} + \tilde{\mu} = \mu \\ \frac{d\tilde{\mu}}{dx} \Big|_{x \rightarrow t} = M, \tilde{\mu}|_{x \rightarrow \infty} = 0 \end{cases} \quad (6.3)$$

where $\tilde{\mu}$ is the filtered density field; M is the given non-homogeneous Neumann boundary condition; r is the length scale of this improved filter which connected with the filter radius field R via the following equation

$$r = \frac{R}{2\sqrt{3}} \quad (6.4)$$

The analytical details of this improved PDE filter can be referred to the research work of Gao et al. (Gao, Yang, Zhang, and Liu, 2023), and according to their derivations, the value of the M can be determined as

$$M = \frac{\sqrt{3}}{R} \quad (6.5)$$

It should be noted that the filter radius field R in this study is a non-uniform field and will be optimized during the TO procedure, which is another significant difference with other researches and is the key for generating the external coating with variable thickness, as presented in Fig. 6.3.

Heaviside projection

Both the PDE-based and the improved PDE-based filters lead to modified density fields with intermediate design variables between 0 and 1, which brings difficulties in the clear identification of the external coating and the infilling area. Therefore, two Heaviside projections are applied toward filtered fields in the proposed two-step filtering and projection procedure for clear black/white designs, as shown in Fig. 6.3. Based on the tangent function, the continuous Heaviside projection with differentiability (Wang, Lazarov, and Sigmund, 2011) can be expressed as follows

$$\bar{X} = \frac{\tanh(\beta\eta) + \tanh(\beta(X - \eta))}{\tanh(\beta\eta) + \tanh(\beta(1 - \eta))} \quad (6.6)$$

where $\bar{X}$ and X are the projected density field and its original field, respectively; β is the sharpness parameter to control the projection effect and Eq. (6.6) becomes the Heaviside step function when β tends to infinity; η denotes the threshold value for the projection, whereby values of the field X greater than η are projected to 1 and others are projected to 0.

Material interpolation functions

Using the techniques outlined above, a new two-step filtering and projection procedure for designing coated structures with non-uniform coating thickness is constructed, as shown in Fig. 6.3, with control parameters indicated. The procedure unfolds as follows: First, the initial design variable field ρ is smoothed using the PDE-based filter (Eq. (6.1)) to produce a filtered density field $\tilde{\rho}$. Next, the first Heaviside projection with parameters β_1 and η_1 is applied to obtain the projected field μ , which serves for coating identification. The μ field is then processed through the improved PDE-based filter (Eq. (6.3)) with a non-homogeneous filter radius R , yielding a filtered density field $\tilde{\mu}$. Finally, the second Heaviside projection is applied to $\tilde{\mu}$ field using parameters β_2 and η_2 (defined as $\eta_2 = 0.5 + \Delta\eta_2$) and a projected field φ is obtained.

Based on the erosion scheme (Luo, Li, and Liu, 2019), the difference between the fields μ and φ is used to define the coating. Specifically, for a certain element e , $\mu_e = 1$ and $\varphi_e = 0$ indicate that the element is occupied by the coating material, while $\varphi_e = 1$ represents the infilling material used. Additionally, $\mu_e = 0$ indicates that it has no solid material and is used for the void domain determination. Therefore, the stiffness and mass functions of the coated structure can be interpolated as

$$\mathbf{E}(\mu, \varphi) = \mu^p (1 - \varphi^p) E_{\text{coating}} + \mu^p \varphi^p E_{\text{infilling}} \quad (6.7)$$

$$\mathbf{M}(\mu, \varphi) = \mu(1 - \varphi)\rho_{\text{coating}} + \mu\varphi\rho_{\text{infilling}} \quad (6.8)$$

where E_{coating} and $E_{\text{infilling}}$ are the Young's modulus and material density for the coating and the infilling, respectively, while ρ_{coating} and $\rho_{\text{infilling}}$ are their material densities. p is the penalty factor to penalize the fields μ and φ for 0/1 solutions, and $p = 3$ is used in the presented study.

According to the derivation in the research of Luo et al. (Luo, Li, and Liu, 2019), the coating thickness field w can be implicitly controlled via the following equation when $\Delta\eta_2 = 0.45$

$$w \approx 1.5R \quad (6.9)$$

6.3 Topology optimization of coated structures

6.3.1 Topology optimization formulations

In this study, the classical optimization problem, i.e., the minimum compliance design, is considered to evaluate the benefits of considering a variable-thickness coating in coated structures and to test the effectiveness of the proposed method. To effectively limit material consumption, two mass constraints are introduced for the optimum design of coated structures, and the mathematical model for compliance minimization can then be formulated as

$$\text{find } \rho, R \quad (6.10a)$$

$$\text{min: } c \quad (6.10b)$$

$$\text{s.t. } \mathbf{K}\mathbf{U} = \mathbf{F} \quad (6.10c)$$

$$G_1 = M - f_1 \cdot M^* \leq 0 \quad (6.10d)$$

$$G_2 = M_{\text{coating}} - f_2 \cdot M^* \leq 0 \quad (6.10e)$$

$$0 < \rho_{\min} \leq \rho_e \leq 1 \quad e = 1, \dots, N \quad (6.10f)$$

$$R_{\min} \leq R_e \leq R_{\max} \quad e = 1, \dots, N \quad (6.10g)$$

where c is the structural compliance; $\mathbf{K}$ is the global stiffness matrix, and $\mathbf{U}$ and $\mathbf{F}$ are the global displacement matrix and the load vector, respectively; M and M_{coating} denote the total mass of the coated structure and the mass of the coating, respectively. M^* is the reference mass value, which equal to the mass of the design domain fully filled with the coating material in this paper; f_1 and f_2 are the maximum allowed mass fractions. The stiffness matrix $\mathbf{K}$ can be obtained using the following equation

$$\mathbf{K} = \sum_e^N E_e(\boldsymbol{\mu}, \boldsymbol{\varphi}) \mathbf{k}_0 \quad (6.11)$$

where $\mathbf{k}_0$ is the elemental stiffness matrix with unit Young's modulus and N is the total number of elements.

Minimum length scale control

During the optimization process, the evolution of the structural topology may lead to some merging of the external coating and no infilling exist (Luo, Li, and Liu, 2019). Therefore, to alleviate this length scale issue, the worst case robust formulation (Sigmund, 2009; Qian and Sigmund, 2013) is introduced into the proposed method to design coated structures due to its simple implementation. Aims at optimizing the structure with the worst structural performance and constraining the mass on the dilated design, the objectives using the worst case robust formulation are respectively modified as

$$c = \max \left(c_1 (\rho^e), c_2 (\rho^i), c_3 (\rho^d) \right) \quad (6.12)$$

where ρ^e , ρ^i , and ρ^d denote the eroded, intermediate, and dilated designs obtained by using the different threshold values $\eta_1^e = 0.5 + \Delta\eta_1$, $\eta_1^i = 0.5$, and $\eta_1^d = 0.5 - \Delta\eta_1$, respectively, for the first Heaviside projection in the two-step filtering and projection procedure.

To effectively control the structural masses, the mass constraints have to be updated during the optimization because they are not directly implemented on the intermediate design and may cause offsets of the structural masses from their prescribed maximum values. For both the mass constraints G_1 and G_2 , the following unified formula can be used for the updates of their mass fractions (f_1 and f_2) at each iteration step:

$$f^* = \frac{M'}{M_i} f \quad (6.13)$$

where f^* denotes the updated mass fraction; M' and M_i mean the prescribed maximum allowed mass of the structure/coating and the mass of the structure/coating at the i -th iteration step, respectively.

6.3.2 Post-processing optimization for generating smooth structural boundaries

In this section, the details of the developed density-based post-processing optimization for coated structures are provided. Functionally, the post-processing optimization inherits the result from the pre-processing optimization stage and targets on achieving smooth structural boundaries, which enables a rapid transformation to CAD models with improved structural performance.

A key part of the post-processing optimization lies in the creation of the body-fitted mesh, which involves generating a new mesh different from the original mesh with smaller elements, that align with the iso-value boundary of an LS surface to better capture geometrical details. Different from other structures, coated structures have two structural boundaries that require smoothing: the inner boundary between the coating and the infilling region, and the outer boundary of the coating. To address both boundaries, the coating identification field is selected as the foundation for

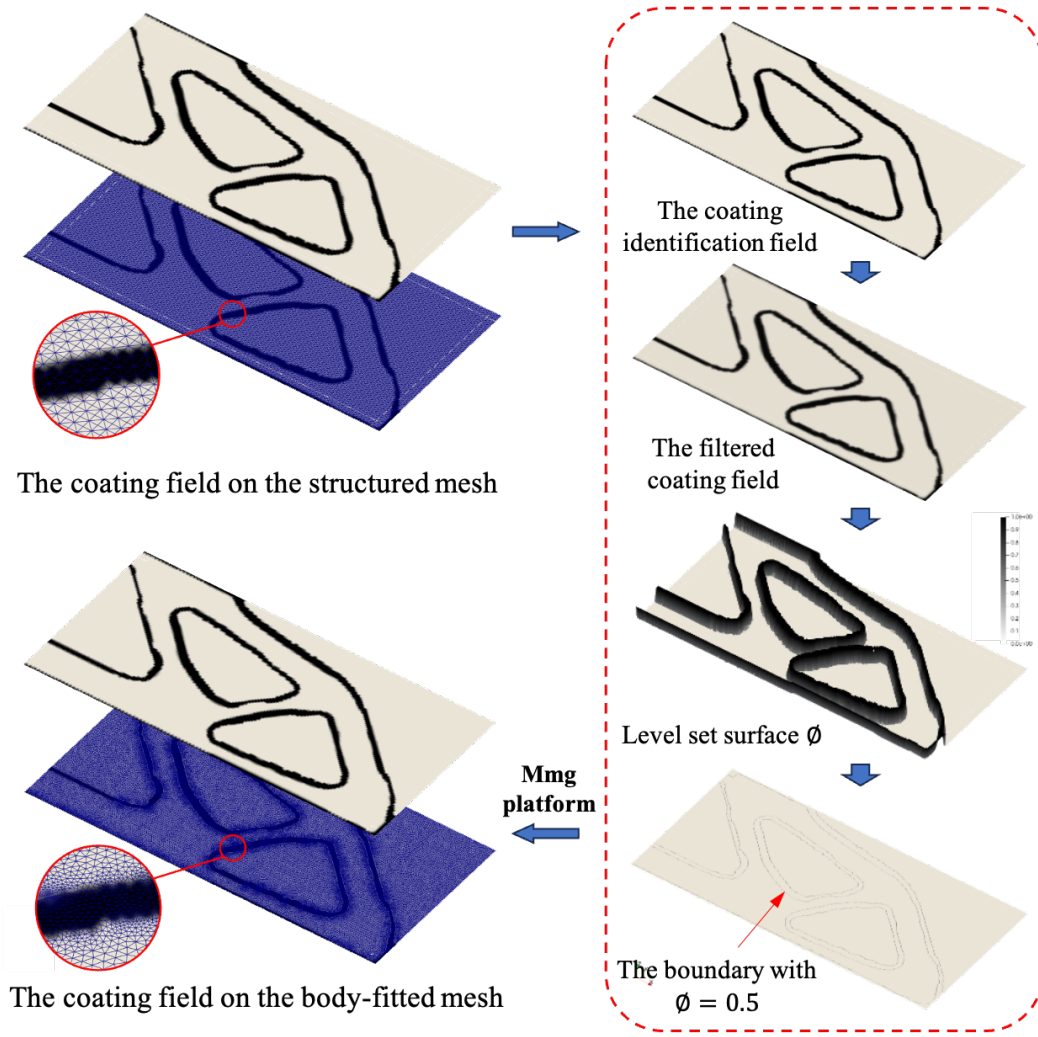


FIGURE 6.4: Illustration on the construction of the body-fitted mesh within the post-processing optimization.

constructing the LS surface because it directly contains the information for both boundaries.

Fig. 6.4 illustrates the procedure for creating the body-fitted mesh in post-processing optimization. Starting with the optimization result from the pre-processing stage on a structured mesh, the coating identification field is firstly extracted for a filtered coating field obtained via another PDE filtering with a homogeneous radius field R_3 . After that, we use this filtered coating field to form a continuous LS surface ϕ ranging from 0 to 1, based on its density values. Then, the iso-surface at $\phi = 0.5$ is used to define the structural boundaries at each iteration step. It should be noted that, in the early stages of post-processing, these boundaries may still retain some dependency on the initial structured mesh and lack full smoothness. However, with local mesh refinement, the boundaries derived from the LS surface progressively become smoother. Next, the design domain is remeshed via the open-source Mmg library (Dapogny, Dobrzynski, and Frey, 2014) employing several control settings (e.g., mesh gradation, maximum and minimum mesh sizes, and boundary approximation controls). Finally, density regularization is performed to create new density

and filter radius fields corresponding to the new mesh with their original values. Especially, the above operations can be achieved with easy implementations, thanks to the powerful function of FreeFEM++ (Hecht, 2012).

The entire optimization of designing coated structures with non-uniform coating and smooth structural boundaries is conducted using the open-source platform FreeFEM++ with the integration of the Mmg platform. As detailed body-fitted mesh construction is beyond the scope of this paper, readers can be directed to the studies by Costa Azevêdo et al. (Costa Azevêdo, Li, Ishida, Siqueira, Cortez, Nelli Silva, Nishiwaki, and Picelli, 2024) and Li et al. (Li, Yamada, Jolivet, Furuta, Kondoh, Izui, and Nishiwaki, 2021) for further information on the Mmg implementation.

6.3.3 Optimization procedure

With the post-processing optimization technique described above, the complete flowchart for the TO of coated structures using the developed approach is shown in Fig. 6.5. This process comprises two stages, i.e., the pre-processing optimization and the post-processing optimization. Functionally, the pre-processing optimization focuses on achieving coated structures with variable coating thickness by optimizing the density field ρ and the non-homogeneous filter radius field R . Once the pre-optimized results are obtained on a fixed mesh, the corresponding data are transferred to the post-processing stage and design variables are further updated, where smooth structural boundaries are generated with the body-fitted mesh construction. The two sets of design variables ρ and R in both the pre-processing and post-processing optimization stages are updated by the method of moving asymptotes (MMA) (Svanberg, 1987) algorithm, due to its excellent optimization capabilities and ability to handle multiple constraints effectively.

The details of the optimization flowchart of the proposed method can be summarized as follows

1. Define the relevant parameters and initialize the structure.
2. Perform the two-step filtering and projection process to obtain filtered and projected fields.
3. Use the modified density fields to identify the coating and infill regions, and interpolate material properties using Eqs. (6.7) and (6.8).
4. Conduct finite element analysis to evaluate the objective function and constraints.
5. If convergence criteria are met, proceed to the post-processing optimization stage (Step 8). If not, calculate the sensitivity information.
6. Update the two sets of design variables using the MMA solver.
7. Return to Step 2.
8. Generate the level set surface using the coating identification field.

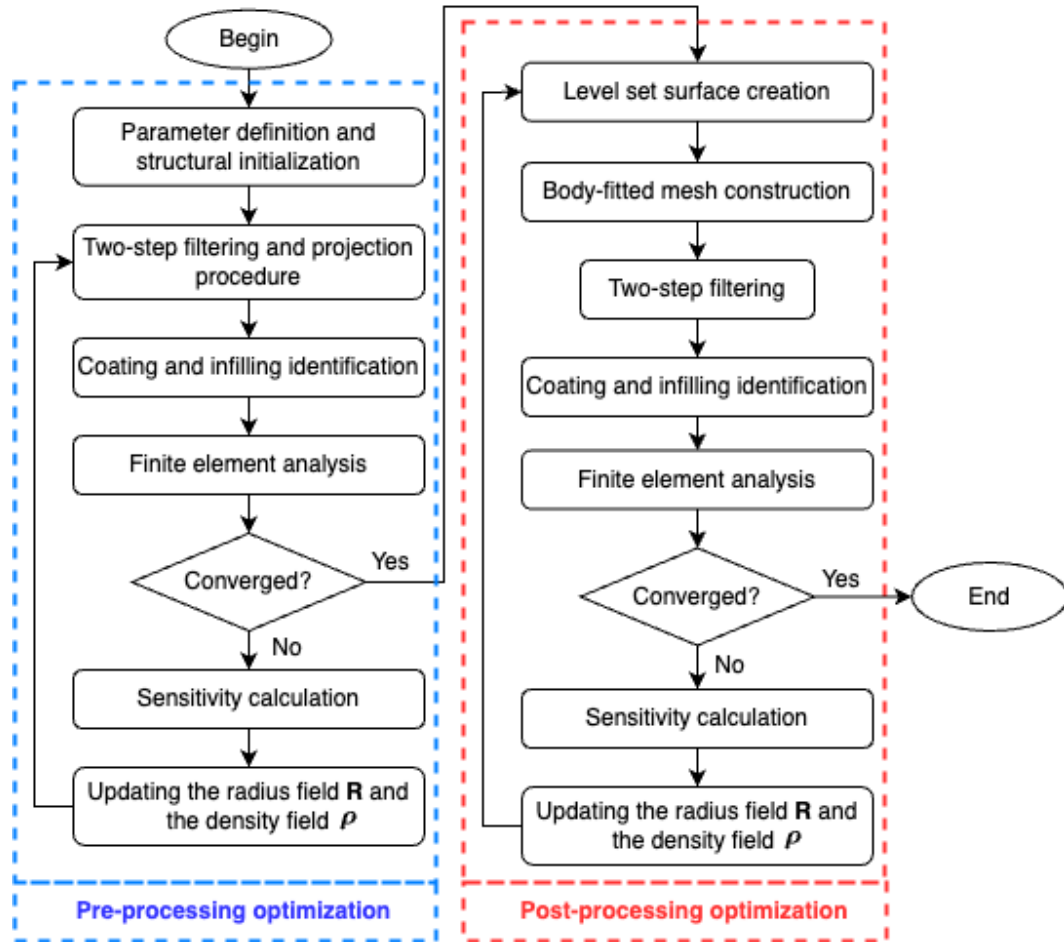


FIGURE 6.5: Optimization flowchart of topology optimization of coated structures with non-uniform coating thickness and smooth structural boundaries using the proposed method.

9. Construct the body-fitted mesh using the Mmg platform.
10. Repeat Steps 2–4 and check the convergence criteria. If met, the optimization concludes with the final optimized coated structure. Otherwise, perform sensitivity analysis and repeat Step 6.
11. Return to Step 8.

To ensure a clear black-and-white solution in the final optimization result, the convergence criteria in Steps (5) and (10) are defined as follows: (1) The sharpness parameter β in the Heaviside projections reaches its maximum value, and (2) the relative difference in objective function values between two consecutive iterations is less than 10^{-4} . The optimization will terminate only when both of these criteria are met.

6.4 Sensitivity analysis

Due to the self-adjoint property of the compliance minimization problem Eq. (6.10), the derivative of the compliance with respect to the density design variable ρ can be expressed as

$$\frac{\partial c}{\partial \rho} = -\mathbf{U}^T \frac{\partial \mathbf{K}}{\partial \rho} \mathbf{U} = -\mathbf{U}^T \frac{\partial \mathbf{E}}{\partial \rho} \mathbf{k}_0 \mathbf{U} \quad (6.14)$$

Based on Eq. (6.7), the term $\frac{\partial \mathbf{E}}{\partial \rho}$ can be derived using the product rule as

$$\begin{aligned} \frac{\partial \mathbf{E}}{\partial \rho} &= p \cdot \mu^{p-1} \frac{\partial \mu}{\partial \rho} [\varphi^p E_{\text{infilling}} + (1 - \varphi^p) E_{\text{coating}}] \\ &+ p \cdot \varphi^{p-1} \mu^p \frac{\partial \varphi}{\partial \rho} [E_{\text{infilling}} - E_{\text{coating}}] \end{aligned} \quad (6.15)$$

Using the chain rule, the terms $\frac{\partial \mu}{\partial \rho}$ and $\frac{\partial \varphi}{\partial \rho}$ in the above equation can be respectively derived as

$$\frac{\partial \mu}{\partial \rho} = \frac{\partial \mu}{\partial \tilde{\rho}} \frac{\partial \tilde{\rho}}{\partial \rho} \quad (6.16)$$

$$\frac{\partial \varphi}{\partial \rho} = \frac{\partial \varphi}{\partial \tilde{\mu}} \frac{\partial \tilde{\mu}}{\partial \mu} \frac{\partial \mu}{\partial \tilde{\rho}} \frac{\partial \tilde{\rho}}{\partial \rho} \quad (6.17)$$

According to Eq. (6.6), the terms $\frac{\partial \mu}{\partial \tilde{\rho}}$ and $\frac{\partial \varphi}{\partial \tilde{\mu}}$ can be calculated using the following formulations

$$\frac{\partial \mu}{\partial \tilde{\rho}} = \beta_1 \frac{1 - \tanh^2(\beta_1(\tilde{\rho} - \eta_1))}{\tanh(\beta_1 \eta_1) + \tanh(\beta_1(1 - \eta_1))} \quad (6.18)$$

$$\frac{\partial \varphi}{\partial \tilde{\mu}} = \beta_2 \frac{1 - \tanh^2(\beta_2(\tilde{\mu} - \eta_2))}{\tanh(\beta_2 \eta_2) + \tanh(\beta_2(1 - \eta_2))} \quad (6.19)$$

With the above equations, the formulation Eq. (6.14) can be successfully calculated to obtain the sensitivity information.

Similarly, the sensitivity of the compliance with respect to the designable filter radius field $\mathbf{R}$ can be expressed as

$$\frac{\partial c}{\partial \mathbf{R}} = -\mathbf{U}^T \frac{\partial \mathbf{K}}{\partial \mathbf{R}} \mathbf{U} = -\mathbf{U}^T \frac{\partial \mathbf{E}}{\partial \mathbf{R}} \mathbf{k}_0 \mathbf{U} \quad (6.20)$$

where the partial derivative $\frac{\partial \mathbf{E}}{\partial \mathbf{R}}$ can be derived according to Eq. (6.7) as the following form

$$\frac{\partial \mathbf{E}}{\partial \mathbf{R}} = p \cdot \mu^p \varphi^{p-1} \frac{\partial \varphi}{\partial \mathbf{R}} [E_{\text{infilling}} - E_{\text{coating}}] \quad (6.21)$$

with the term $\frac{\partial \varphi}{\partial R}$ derived as

$$\frac{\partial \varphi}{\partial R} = \frac{\partial \varphi}{\partial \tilde{\mu}} \frac{\partial \tilde{\mu}}{\partial R} \quad (6.22)$$

It should be noted that the term $\frac{\partial \tilde{\mu}}{\partial R}$ in the above equation is unknown and should be derived. Here, due to the space limitation, how to calculate the term $\frac{\partial \tilde{\mu}}{\partial R}$ is provided in the Appendix A with details described.

Based on the above equations and Eq. (6.8), the sensitivities of the mass constraints G_1 and G_2 with respect to design variable ρ can also be derived as follows

$$\begin{aligned} \frac{\partial G_1}{\partial \rho} &= \frac{\partial \mu}{\partial \rho} [(1 - \varphi)\rho_{\text{coating}} + \varphi\rho_{\text{infilling}}] \\ &\quad + \frac{\partial \varphi}{\partial \rho} \mu (\rho_{\text{infilling}} - \rho_{\text{coating}}) \end{aligned} \quad (6.23a)$$

$$\frac{\partial G_2}{\partial \rho} = \frac{\partial \mu}{\partial \rho} (1 - \varphi)\rho_{\text{coating}} - \frac{\partial \varphi}{\partial \rho} \mu \rho_{\text{coating}} \quad (6.23b)$$

Similarly, for the designable filter radius field R , the sensitivity equations are written as

$$\frac{\partial G_1}{\partial R} = \frac{\partial \varphi}{\partial R} \mu (\rho_{\text{infilling}} - \rho_{\text{coating}}) \quad (6.24a)$$

$$\frac{\partial G_2}{\partial R} = -\frac{\partial \varphi}{\partial R} \mu \rho_{\text{coating}} \quad (6.24b)$$

6.5 Numerical examples

In this section, several numerical examples are provided to verify the effectiveness of the proposed method. In order to improve the convergence behavior of the algorithm, the sharpness parameters β_1 and β_2 are linked as $\beta_1 = \beta_2$, and are gradually increased by doubling them at every 100 iteration steps from 1 to 128. For all numerical examples, the material properties for the coating and the infilling region are set as $E_{\text{coating}} = 1$, $\rho_{\text{coating}} = 1$, and $E_{\text{infilling}} = 0.6$, $\rho_{\text{infilling}} = 0.8$.

6.5.1 Considering uniform and non-uniform coating thickness

As the first numerical example, we examine the advantages and effectiveness of incorporating the non-uniform coating thickness in the optimum design of coated structures. A cantilever beam, with its geometrical dimensions and boundary shown in Fig. 6.6, is optimized with uniform and non-uniform coating thickness to provide a comparison. The mass constraints are applied as $f_1 = 40\%$ and $f_2 = 15\%$, respectively. For the uniform coating case, the coating thickness is set as $w = 3$ and the filter radius field R is homogeneous (i.e., $R = 4.5$ via Eq. (6.9)). As for the

non-uniform coating case, the maximum and minimum values for the non-homogeneous filter radius field R are defined as $R_{\min} = 1.5$ and $R_{\max} = 7.5$ (i.e., $w_{\min} = 1$ and $w_{\max} = 5$). To clearly visualize the optimization results at two stages using the developed approach, the pre-optimized and post-optimized results are both presented.

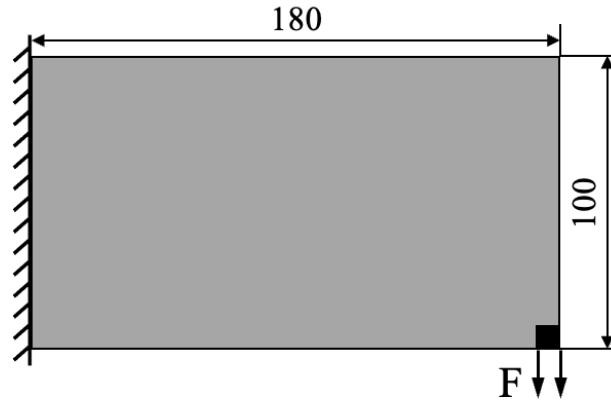


FIGURE 6.6: Structural representation of the cantilever beam.

Fig. 6.7 shows the optimized cantilever beam considering the uniform coating thickness. As can be seen, the pre-optimized and post-optimized results share the same structural topology. However, compared to the zig-zag boundaries shown in Fig. 6.7a, the post-optimized cantilever beam shown in Fig. 6.7b has smooth structural boundary representation, which proves the effectiveness of the post-processing optimization in generating smooth structural boundaries. The zoomed out figures in Fig. 6.7 offer more details. Obviously, the post-optimized result is based on the body-fitted mesh, rather than the structured mesh for the pre-processing optimization, which greatly adapt to the structural geometry with both inner and outer boundaries smoothly demonstrated.

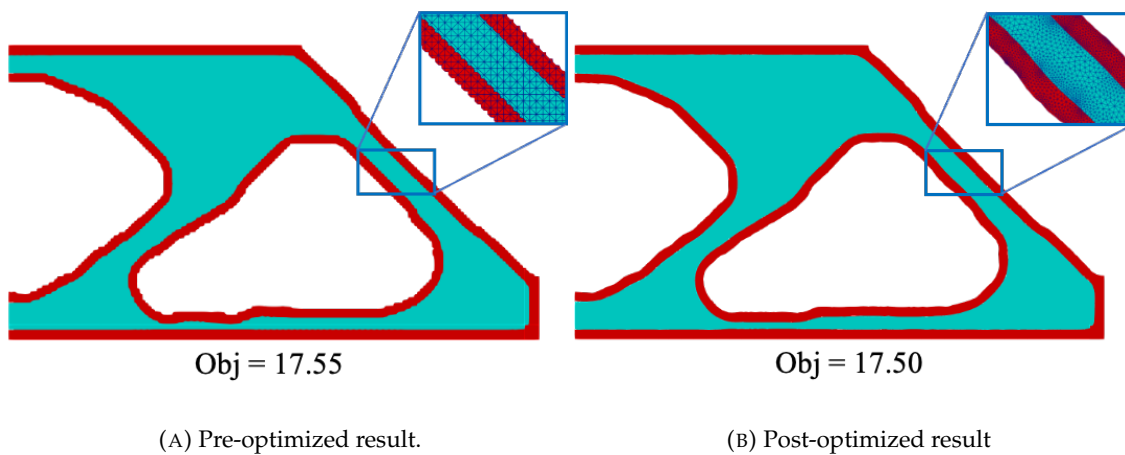


FIGURE 6.7: Optimization results of the cantilever beam with uniform coating thickness.

For the coated cantilever beam with non-uniform coating thickness, the pre-optimized and post-optimized designs presented in Fig. 6.8 retain the same structural topology. However, certain differences emerge between the topologies of the uniform coating and non-uniform coating cases, highlighting the impact of variable coating thickness on the final design. The final result obtained via the post-processing optimization as shown in Fig. 6.8b still exhibit much smoother structural boundaries than the pre-optimized result shown in Fig. 6.8a. Same as the uniform coating case, the body-fitted mesh for the post-optimized cantilever beam also greatly fits the structural boundaries and the geometry is well described.

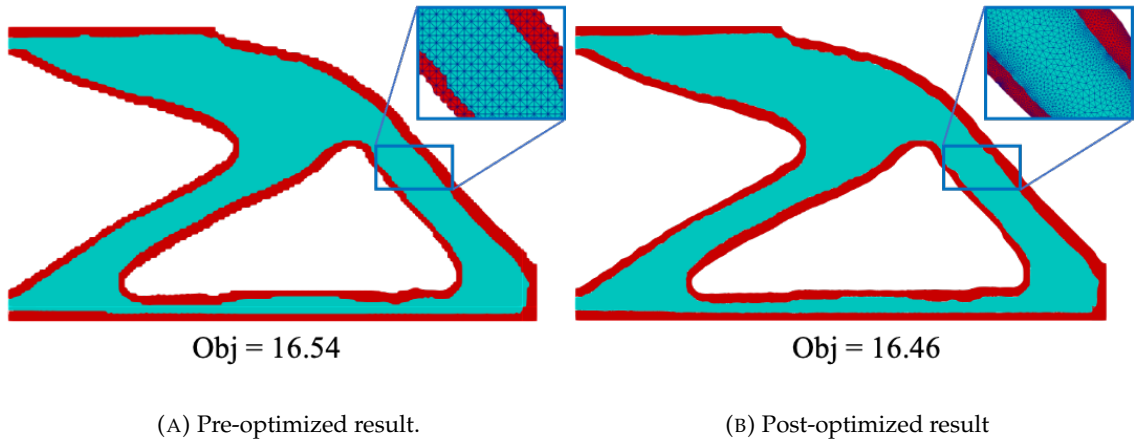


FIGURE 6.8: Optimization results of the cantilever beam with non-uniform coating thickness.

It can be observed that the coating with variable thickness is successfully achieved in the non-uniform coating case, as shown in Fig. 6.8. Generally, the coating near the left edge of the cantilever beam has larger thickness to better resist the external force, as well as the outer coating on the right inclined edges. As for the uniform coating case, the coating maintains a consistent thickness throughout. The final objective function values for cantilever beams considering uniform and non-uniform coating thickness are 17.50 and 16.46, respectively. This indicates an approximate 6% improvement in structural performance when a variable coating thickness is applied. In addition, we find that the post-processing optimization stage with body-fitted mesh construction can further improve the structural stiffness in both cases, leading 0.30% and 0.48% decrement on compliance values, respectively.

The iteration histories of the optimization considering uniform and non-uniform coating thickness are shown in Fig. 6.9 and Fig. 6.10, respectively. As can be seen, the objective function and mass fractions of the structures have certain ups and downs during the early stage in both cases. However, the iteration histories of the pre-processing optimization gradually become stable with the growth of the iteration number and reach their maximum allowed mass fractions till the maximum iteration step. Several significant fluctuations on the structural masses can be observed both

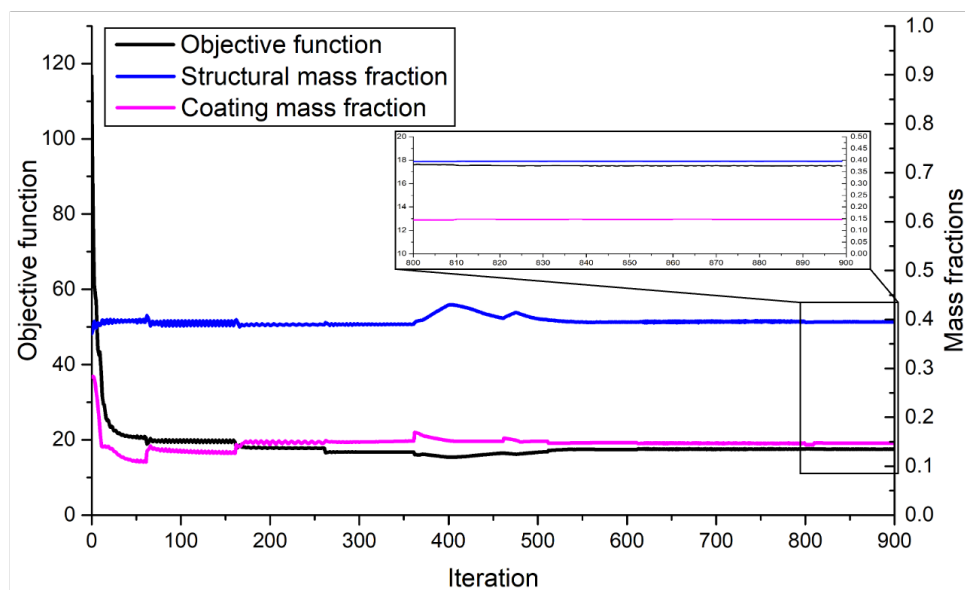


FIGURE 6.9: Iteration history of the TO process for the cantilever beam with uniform coating thickness.

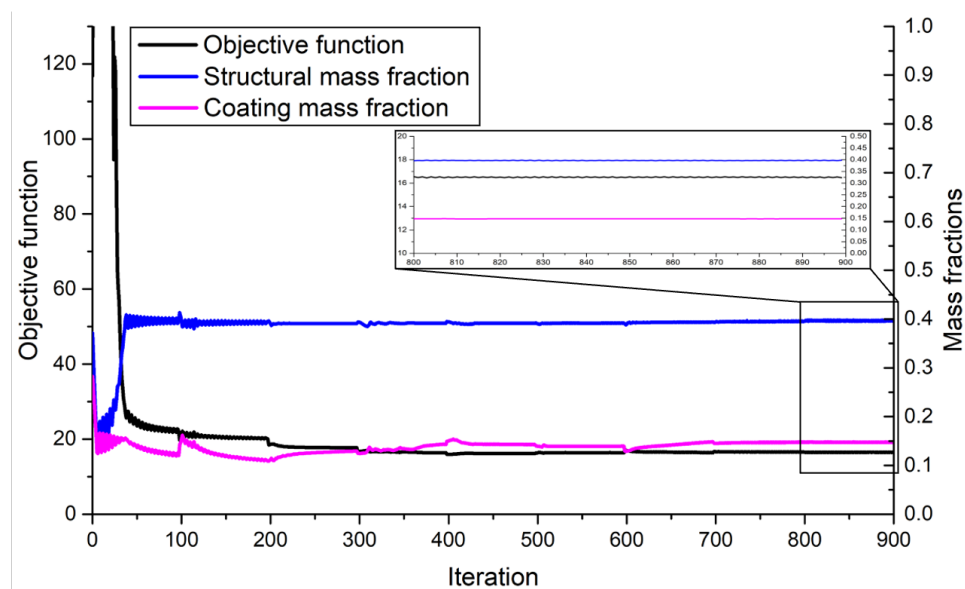


FIGURE 6.10: Iteration history of the TO process for the cantilever beam with non-uniform coating thickness.

in Fig. 6.9 and Fig. 6.10 during the pre-processing stage, which are caused by the huge structural transformation because of the updating of the corresponding sharpness parameters β_1 and β_2 for Heaviside projections. But generally, the pre-processing optimization still exhibit great convergence behavior. The iteration history of the post-processing optimization stage considering the uniform coating thickness, as presented in zoom out figure in Fig. 6.9, has a small increment on its objective function at the first 10 steps, but slowly become steady till the end of the optimization. For the non-uniform coating case, all the iteration curves for the objective function and mass constraints shown in Fig. 6.10 exhibit pretty stable performance during the post-processing optimization and both maximum allowed mass fractions are reached, which proves the effectiveness of the introduced post-processing optimization in handling multiple constraints.

Through this examples, it can be concluded that coated structures optimized with consideration of a non-uniform coating can lead to better structural performance than those designed with uniform coating thickness. Besides, the developed TO method has pretty stable iteration performance and the post-processing optimization stage has great ability to achieve smooth structural representation with enhanced structure performance.

6.5.2 Considering different mass fractions

Next, we test the influence of different mass fractions on the final optimization results with variable coating thickness. Since two mass constraints are introduced in the developed method, three cases of different mass constraints are considered in this subsection: (a) Case A: $f_1 = 40\%$, $f_2 = 15\%$; (b) Case B: $f_1 = 50\%$, $f_2 = 15\%$; and (c) Case C: $f_1 = 40\%$, $f_2 = 20\%$. The maximum and minimum values for the filter radius are kept the same as the previous example.

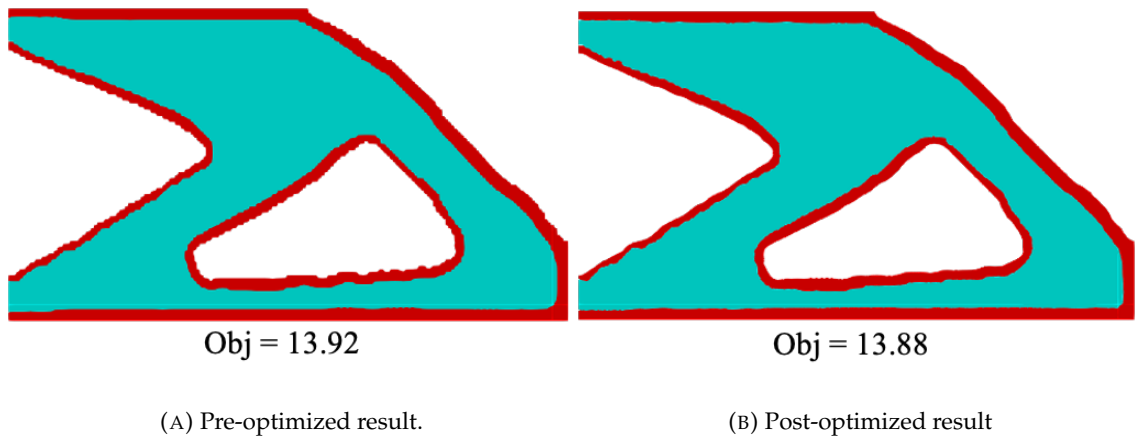


FIGURE 6.11: Optimization results of the cantilever beam with non-uniform coating thickness considering the mass constraints of Case B.

The pre-optimized and post-optimized results for Case A have already been presented in Fig. 6.8.

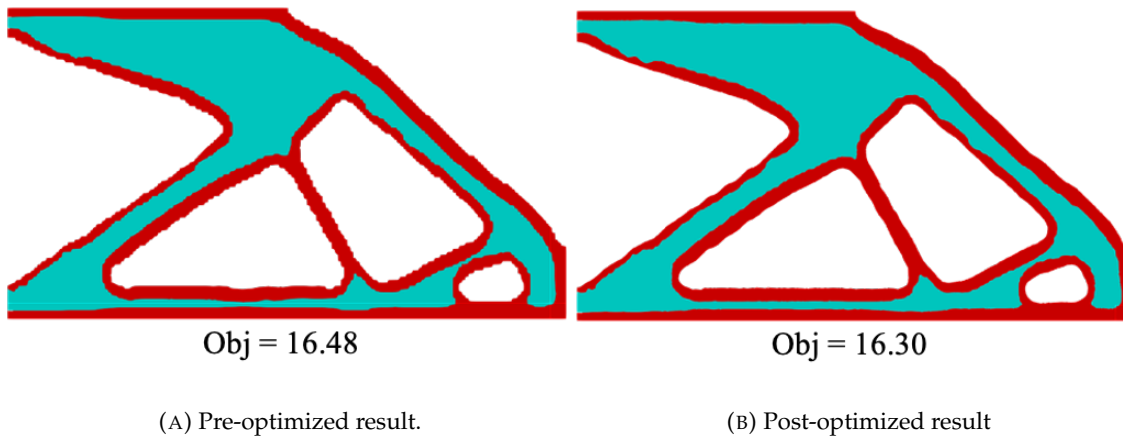


FIGURE 6.12: Optimization results of the cantilever beam with non-uniform coating thickness considering the mass constraints of Case C.

For Case B, the corresponding results are shown in Fig. 6.11, with the objective function values labeled as 13.92 and 13.88, respectively. And Fig. 6.12 illustrates the optimized cantilever beam using the Case C mass constraints, with objective function values as 16.48 and 16.30, respectively. Still, the post-optimized results in both Case B and C own a better structural performance with smooth structural boundaries achieved, which proves the effectiveness of the developed post-processing optimization stage.

Under the same mass constraint applied on the coating, the structural topologies shown in Fig. 6.8 and Fig. 6.11 have great similarities. In addition, it can be found that the thickness distribution of the coating in Cases A and B also demonstrate the same tendency. With significant difference, optimization results in Fig. 6.12 present a new structural topology with more coating material demonstrated due to a larger coating mass fraction applied. Generally, the results for Case C shown in Fig. 6.12 have higher compliance values than those in Case B but are marginally lower than those observed in Case A. In the authors' view, this phenomenon indicates that the total mass constraint could play a dominant role in determining the structural performance, rather than the coating mass constraint.

Through this numerical example, we find that the developed TO algorithm can effectively deal with different mass constraints and smooth structural boundaries with better performance can always achieved using the developed optimization procedure. Moreover, applying different mass constraints has the ability to build varied structural topologies.

6.5.3 Considering different maximum and minimum values for R

In this subsection, we test how the maximum and minimum values for the non-homogeneous filter radius field R will affect the final optimization results. A clamped ends beam model is

selected for the corresponding tests and its geometrical dimensions are illustrated in Fig. 6.13. Three cases of different maximum and minimum values for the non-homogeneous filter radius field R are considered: (a) Case A: $R_{\min} = 1.5$ and $R_{\max} = 3.0$ ($w_{\min} = 1$ and $w_{\max} = 2$), (b) Case B: $R_{\min} = 1.5$ and $R_{\max} = 4.5$ ($w_{\min} = 1$ and $w_{\max} = 3$), and (c) Case C: $R_{\min} = 3.0$ and $R_{\max} = 4.5$ ($w_{\min} = 2$ and $w_{\max} = 3$). The mass constraints are set as $f_1 = 50\%$, $f_2 = 15\%$. Similarly, both the pre-optimized and the post-optimized results in all cases are presented to offer more details of the optimization process.

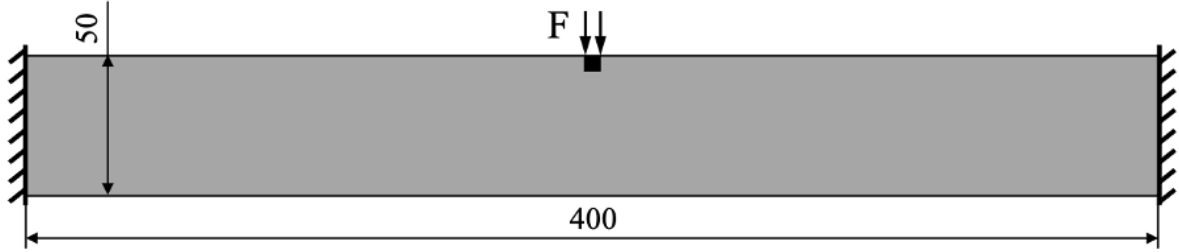


FIGURE 6.13: Structural representation of the clamped ends beam.

Fig. 6.14 shows the optimization results considering Case A ($R_{\min} = 1.5$ and $R_{\max} = 3.0$), with objective function values of them as 83.37 and 82.75, respectively. As can be observed, the pre-optimized and the post-optimized results still share the same structural topology. However, the post-optimized result shown in Fig. 6.14b exhibits smooth structural boundaries with a smaller objective function value, revealing the effectiveness of the post-optimization stage.

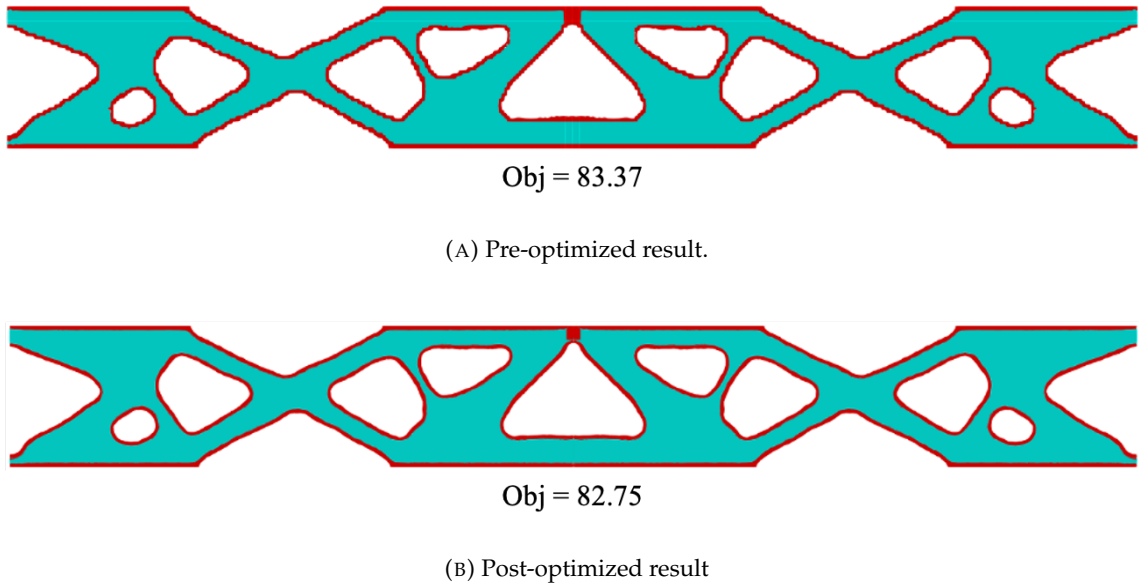


FIGURE 6.14: Optimization results of the clamped ends beam considering different values for R of Case A.

For the second case of the tests, optimization results are presented in Fig. 6.15. Compared to

Case A ($R_{\min} = 1.5$ and $R_{\max} = 3.0$), a larger value of the term $R_{\max}$ lead to no change on the topology of optimized results in this case. However, it can be seen that both results for Case B in Fig. 6.15 have a coating with larger thickness. With a larger difference between the values of $R_{\min}$ and $R_{\max}$, the optimization problem owns a larger design freedom and the optimized coating has obvious varied thicknesses. Generally, the outer coating near the fixed boundaries exhibits greater thickness and show small thickness at the central area of the structure. The objective function values of two results are 80.36 and 79.62. Still, the post-optimization stage still leads to better structural performance with smooth structural representation.

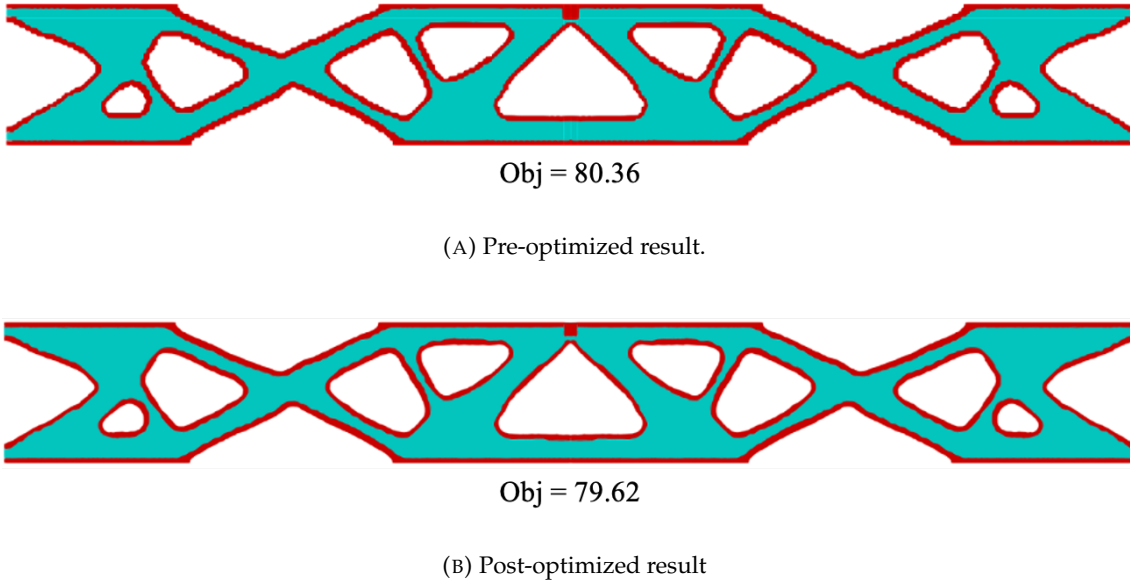


FIGURE 6.15: Optimization results of the clamped ends beam considering different values for R of Case B.

Fig. 6.16 shows the optimization results of the final test case. With a larger value of $R_{\min}$, a new structural topology for Case C with less trusses is obtained. As introduced before, varied values of R can lead to varied coating thicknesses. Therefore, the generation of this new topology is created because of the coating evolution during the optimization process, revealing the interaction effect between the structural evolution and the coating generation. The pre-optimized result presented in Fig. 6.16a shows obvious zig-zag boundaries and the one obtained via the post-processing stage has pretty smooth structural outlines. Also, the post-optimized one still has better structural performance than its pre-optimized one.

With these numerical results, it can be concluded that the pre-defined maximum and minimum values for the non-homogeneous filter radius field R have certain influence on the final topology and structural performance. Besides, among the considered three cases, a slight adjustment to the maximum and minimum values of R can result in approximately a 4% improvement in structural performance. Therefore, designers should carefully set these values before the optimization to better develop the potential of material and coated structure. Moreover, the setting of $R_{\min}$ should

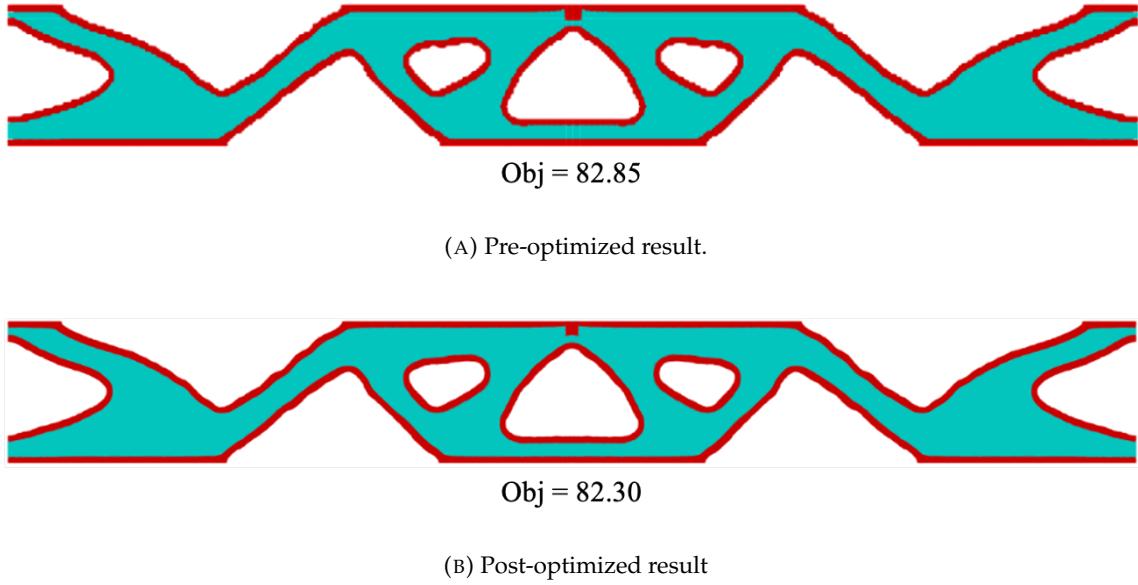


FIGURE 6.16: Optimization results of the clamped ends beam considering different values for R of Case C.

also considers the minimum printing parameter of AM machines for a successful manufacturing. The effectiveness of the proposed method is still greatly proved in this numerical test, with expected non-uniform coating thickness and smooth structural representation achieved.

6.6 Conclusions

This paper investigates the optimum design of coated structures and proposes a novel density-based TO method for achieving non-uniform coating thickness and smooth structural boundaries of coated structures. Based on the standard two-step filtering and projection procedure, an improved PDE-based filter is for coating identification, addressing boundary effects, and simplifying the modeling process. By treating the filter radius field of the improved PDE filter as a design variable, the coating thickness can be tailored to better resist the external force, enabling an external coating with variable thickness. Following the pre-optimized result using the structured mesh, a post-processing optimization is implemented to generate smooth structural boundaries using the body-fitted mesh, with further optimization on design variables. Numerical examples verify that the developed approach possesses the following remarkable features: (1) The coated structures optimized using the proposed method have better structural performance than those designed with uniform coating thickness; (2) Results obtained via the post-processing density-based optimization stage exhibit smooth structural boundary representation and have better structural performance than their pre-optimized ones; (3) The developed method can effectively deal with multiple constraints thanks to the implementation of gradient-based mathematical algorithm; (4)

Both the pre-processing and post-processing optimization stages demonstrate stable iteration performance, revealing the proposed TO method has great convergence behavior; (5) The numerical range of the non-homogeneous filter radius field has certain influence on both the structural performance and the structural topology.

Although this study focuses on the compliance minimization problem, it would be highly valuable to extend the proposed method for designing coated structures with non-uniform coating thickness and smooth structural boundaries to other applications. Examples include the dynamic TO of multiscale coated structures and the bionic design of bone tissue scaffolds, which will be investigated by us in the near future.

Chapter 7

General Conclusions

This thesis focuses on the optimum design of coated structures and explores several strategies, including multiscale TO, multi-material design, dynamic structural performance, and non-uniform coating thickness. The following is a summary of achievements.

In Chapter 2, a novel multiscale TO framework for designing coated structures infilled with layer-wise lattice microstructures is developed, and the eigenfrequency maximization problem is solved using the developed method. That is, the macroscale structure is optimized using the velocity field-based level set (VFLS) method, whose infilling region is uniformly (or near uniformly) divided into several layers, and each layer is composed of the periodic distribution of a certain microstructure designed via the popular density method. Due to the inheritance of the implicit geometrical representation and signed distance property of the conventional level set (LS) method, the VFLS method has the ability to generate smooth structural boundaries and greatly maintain the uniform thickness of the outer coating. The asymptotic homogenization method is used to calculate the effective material properties of microstructures, which bridges macroscale and microscale structural designs. The modal assurance criteria (MAC) method is introduced to handle multiple eigenfrequencies, and its effectiveness and advantages are proved. With higher design flexibility, it is found that coated structures with layer-wise graded lattice infill have higher eigenfrequencies than those with periodic and uniform lattice infill microstructures. The influence of layers of lattice infill and coating thickness on the concurrent optimization of macrostructures and microstructures are carefully studied by showcasing several numerical examples, and the usefulness of the proposed method is also confirmed, as well as the manufacturability of optimization results.

In Chapter 3, the above multiscale TO framework is extended to minimum dynamic compliance design under time-harmonic excitation force. Differently, the microstructures for the substrate of coated structures are bi-material, which can enlarge the design space and better resist the vibration response. Apart from two volume constraints to limit the material consumption at two scales, a static compliance constraint is also introduced into the mathematical model to ensure the connectivity of material layout of coated structures when an excitation frequency higher than the

fundamental eigenfrequency is applied. Thanks to the employment of a general mathematical programming algorithm, such a multiple-constraint optimization can be effectively performed by the VFLS method. The sensitivity analysis for the dynamic compliance with respect to the design variables at different scales is carefully performed and the influences of the number of divided layers, excitation frequency, coating thickness, damping coefficients, element meshes, static constraint, and division direction for the lattice infill on the optimized macroscale and microscale structures are studied by several numerical examples. Moreover, a body-fitted mesh for a Computer-Aided Design (CAD) model is constructed and the finite element analysis results further verify the effectiveness of the proposed approach.

In Chapter 4, a novel TO method for the design of coated structures infilled with multiple materials is proposed, where a new material interpolation model for the TO is developed based on the ordered solid isotropic material with penalization (SIMP) scheme. With the introduction of two special Heaviside projections into the two-step filtering and projection procedure, the external coating and the substrate region can be well identified by using several modified design variables. Then, the material distribution of the multi-material infilling is obtained by multiplying the infilling identification field with the piece-wisely projected design variables and optimized via the mathematical programming algorithm under the ordered SIMP framework. Using an eroded density field and its original field, the uniform thickness of the external coating can be effectively controlled. The proposed approach for optimizing coated structures with multi-phase infill materials is easy to implement due to its implementation relying on those frequently-used filtering and projection operations. Besides, without introducing any additional design variables, the developed method inherits the advantages of the ordered SIMP method and has great calculation efficiency and stable iteration performance. With the consideration of several issues such as different coating thicknesses and different design parameters, several 2D numerical examples are studied to demonstrate the effectiveness of the proposed approach, as well as a 3D numerical example optimized using the parallel computing. The optimization results illustrate that the developed method is effective for the design of coated structures infilled with multiple materials and the advantages of considering multiple infill materials is also validated.

In Chapter 5, designing coated structures infilled with multiple self-connected lattice microstructures by extending the above approach to the multiscale static compliance problem is developed. Specifically, the macroscale distribution of multiple infilling materials is replaced by certain microstructural configurations optimized using the TO technique. The numerical homogenization method is also used to calculate the homogenized material properties of microstructures for the macroscale finite element analysis (FEA). To conveniently ensure the connectivity between different microstructural configurations, the designable connective region (DCR) method is introduced into the proposed approach to achieve the self-connected property of optimized lattice microstructures. The effectiveness of the proposed method is proved through several numerical examples, with discussions on the influences of different coating thicknesses, different volume fractions, etc.

In addition, the manufacturability of optimized structures at two scales is also illustrated by using the additive manufacturing (AM) technique, which further validates the applicability of the proposed approach.

In Chapter 6, the non-uniform coating thickness and smooth structural boundaries of coated structures are achieved by developing a new density-based TO method. An improved PDE filter with non-homogeneous Neumann boundary conditions, rather than the original PDE filter with Dirichlet boundary conditions, is introduced into the classical erosion-based procedure to address the boundary effect issue, which can simplify the modeling process with no need to construct the extended area of the design domain. To achieve the non-uniform coating thickness, the filtering radius of the second PDF filtering in the two-step filtering is also selected as the design variable, and is concurrently optimized with the density field for the structural evolution of coated structures. After getting a clear structural topology, a level set surface is constructed via the linear transformation of the coating identification field, and the body-fitted mesh is created. Then, a post-processing optimization to further optimize those two kinds of design variables for better structural performance is conducted, with the generation of smooth structural boundaries. Numerical results prove the effectiveness of the proposed method and verify that considering non-uniform coating thickness can lead to better structural performance.

To conclude, this thesis constructed both the theoretical foundations and computational algorithms for the TO of coated structures, addressing multiple scales, diverse materials, dynamic structural performance, and variable coating thickness. The methods and optimization frameworks presented in this thesis, implemented using density or level set approaches, aim to enable advancement in the optimum design of coated structures and motivate innovative real-world applications of this novel structural configuration.

Appendix A

Calculation of the term $\frac{\partial \tilde{\mu}}{\partial R}$

In this section, we describe the details on how to calculate the partial differential term $\frac{\partial \tilde{\mu}}{\partial R}$ in Eq. (6.22). To begin with, we multiply both sides of the improved PDE-based filter Eq. (6.3) by a test function v and integrate over the domain Ω :

$$-r^2 \int_{\Omega} v \cdot \nabla^2 \tilde{\mu} d\Omega + \int_{\Omega} v \tilde{\mu} d\Omega = \int_{\Omega} v \mu d\Omega \quad (\text{A.1})$$

Then, using the integration by parts, the above equation can be further re-written as

$$\int_{\Omega} v \cdot \nabla^2 \tilde{\mu} d\Omega = \int_{\partial\Omega} v \frac{\partial \tilde{\mu}}{\partial \mathbf{n}} dS - \int_{\Omega} \nabla v \cdot \nabla \tilde{\mu} d\Omega \quad (\text{A.2})$$

where $\partial\Omega$ denotes the boundary of the domain Ω . Due to the boundary condition $\frac{\partial \tilde{\mu}}{\partial \mathbf{n}} = M$, the following formulation can be obtained

$$\int_{\partial\Omega} v \frac{\partial \tilde{\mu}}{\partial \mathbf{n}} dS = \int_{\partial\Omega} M v dS \quad (\text{A.3})$$

Therefore, Eq. (A.2) can be further derived as

$$\begin{aligned} r^2 \int_{\Omega} \nabla v \cdot \nabla \tilde{\mu} d\Omega - r^2 \int_{\partial\Omega} M v dS + \int_{\Omega} v \tilde{\mu} d\Omega \\ - \int_{\Omega} v \mu d\Omega = 0 \end{aligned} \quad (\text{A.4})$$

For simplicity, we record the term $\frac{\partial \tilde{\mu}}{\partial R}$ as ψ and r^2 as ξ . Then, the above equation can be re-written as following equation

$$\begin{aligned} \int_{\Omega} \xi(\mathbf{R}) \nabla \tilde{\mu}(\mathbf{R}) \cdot \nabla v d\Omega - \int_{\partial\Omega} \xi(\mathbf{R}) M v dS \\ + \int_{\Omega} \tilde{\mu}(\mathbf{R}) v d\Omega - \int_{\Omega} \mu v d\Omega = 0 \end{aligned} \quad (\text{A.5})$$

Considering the partial differential of the above equation with respect to the designable filter radius field R , we can obtain the following equation

$$\begin{aligned} & \int_{\Omega} \xi(R) \nabla \psi \cdot \nabla v d\Omega + \int_{\Omega} 2r \frac{\partial r}{\partial R} \nabla \tilde{\mu} \cdot \nabla v d\Omega \\ & + \int_{\Omega} \psi v d\Omega - \int_{\partial\Omega} 2r \frac{\partial r}{\partial R} M v dS = 0 \end{aligned} \quad (\text{A.6})$$

Finally, the formulation to calculate the term ψ (i.e., $\frac{\partial \tilde{\mu}}{\partial R}$) can be obtained as

$$\begin{aligned} & \int_{\Omega} r^2 \nabla \psi \cdot \nabla v d\Omega + \int_{\Omega} \frac{r}{\sqrt{3}} \nabla \tilde{\mu} \cdot \nabla v d\Omega \\ & + \int_{\Omega} v d\Omega - \int_{\partial\Omega} \frac{r}{\sqrt{3}} M v dS = 0 \end{aligned} \quad (\text{A.7})$$

With Eq. (A.7), the sensitivity for updating the designable filter radius field R can be obtained and the optimization for coated structures with non-uniform coating thickness can be conducted.

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Publication List

Peer-reviewed Journal Articles

1. **Hu, T.**, Wang, Y., Furuta, K., Izui, K., and Nishiwaki, S., "Density-based topology optimization of coated structures with non-uniform coating thickness and smooth structural boundaries." Preprint submitted to *Structural and Multidisciplinary Optimization* (2025), under review.
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Conference Presentations

1. **Hu, T.**, Wang, Y., Furuta, K., Izui, K., and Nishiwaki, S., "Topology optimization of coated structures infilled with multiple self-connected microstructures." *26th International Congress of Theoretical and Applied Mechanics (ICTAM-2024)*, Daegu, Korea, Aug 25–Aug 30, 2024.
2. **Hu, T.**, Furuta, K., Izui, K., and Nishiwaki, S., "Multiscale topology optimization of coated structures with multiple self-connected infilling microstructures." *Asian Congress of Structural and Multidisciplinary Optimization 2024 (ACSMO-24)*, Zhengzhou, China, May 19–May 23, 2024.
3. **Hu, T.**, Wang, Y., Zhang, H., Li, H., Furuta, K., Izui, K., and Nishiwaki, S., "Concurrent multiscale topology optimization of coated structures infilled with layer-wise lattice microstructures for dynamic structural performance." *15th World Congress of Structural and Multidisciplinary Optimization (WCSMO-15)*, Cork, Ireland, June 5–June 9, 2023.
4. **Hu, T.**, Wang, Y., Zhang, H., Li, H., Ding, X., Izui, K., and Nishiwaki, S., "Multiscale topology optimization of coated structures with layer-wise graded lattice infill for maximum fundamental eigenfrequency." *Design & Systems conference 22*, Okayama, Japan, Sep 20–Sep 22, 2022.
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6. **Hu, T.**, Ding, X., Zhang, H., and Shen, L., "Stiffener layout optimization for three-dimensional box structures with maximization of natural frequencies." *14th World Congress of Structural and Multidisciplinary Optimization (WCSMO-14)*, Boulder, USA, June 13–June 18, 2021.
7. Li, H., Ding, X., and **Hu, T.**, "Optimal design and thermal modeling for liquid-cooled heat sink based on multi-objective topology optimization: an experimental and numerical study." *13th World Congress of Structural and Multidisciplinary Optimization (WCSMO-13)*, Beijing, China, May 20–May 24, 2019.