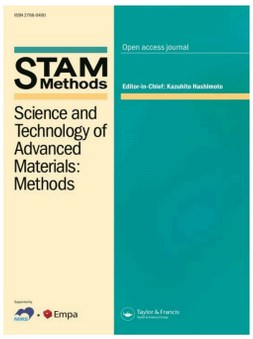

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Computational microstructure design for mechanical property optimization: a review

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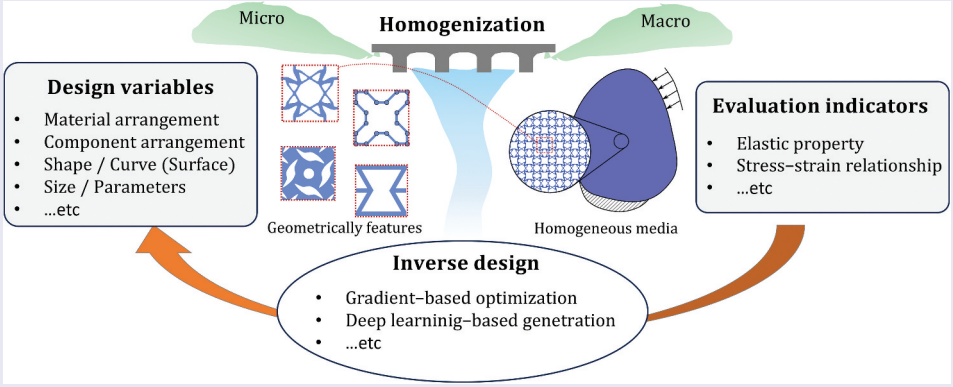
ABSTRACT

The intricate geometrical features of microstructures are key to achieving novel macroscopic structural properties. Recently, mechanical metamaterials, known for exhibiting mechanical properties that surpass those of natural materials, have drawn significant attention. Determining their optimal microstructural morphology to achieve desired mechanical properties is challenging, necessitating advanced computational design techniques. Concurrently, manufacturing technology must advance to produce these increasingly complex microstructures with high fidelity. This review specifically examines the interrelationship between structure and property within the broader process – structure – property – performance reciprocity framework of material design. We comprehensively categorize and present computational methods for both forward and inverse design problems. As computational design methods progress, mechanical metamaterials, already applied in fields such as soft robotics, medical devices, and aerospace, are expected to evolve dramatically into more advanced functional materials. We also address challenges and future prospects in microstructure fabrication, explicitly incorporating process considerations. This paper aims to provide valuable insights for all researchers involved in materials design with a focus on microstructural heterogeneity, irrespective of their primary engagement with computational methods.



IMPACT STATEMENT

This review integratively analyzes theory-based (e.g., topology optimization) and data-driven (e.g., deep generative modeling) computational design methods for mechanical microstructures within a unified framework, discussing manufacturing challenges and future perspectives.

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1. Introduction

Heterogeneous microstructures possess distinct geometric features that dictate macroscopic material properties [1]. Various measurement techniques have been proposed to elucidate the relationships between these geometric features and material properties. These material heterogeneities span a wide range of length scales, from nanoscale molecular structures to microscale features. While the plasticity and bonding states of atoms and molecules determine the intrinsic properties, heterogeneity at larger scales significantly influences overall material behavior. Interpreting such complex heterogeneities poses significant challenges, historically leading to their simplified representation.

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Nevertheless, the ability to manipulate these heterogeneities across multiple scales is paramount for the creation of innovative materials.

The intricate interrelationships among process, structure, property, and performance are fundamental to the materials design paradigm [2,3]. In contrast to traditional materials development, which often relied on empirical correlations between processing and properties, this paradigm integrates principles from systems engineering and computational science. This integration facilitates the rational design of materials with precisely tailored quantitative properties.

Large-scale national and international initiatives are actively exploiting material heterogeneity for the creation of novel materials. In Japan, a prominent initiative was the Japan Science and Technology Agency (JST) project, 'Heterogeneous Structure Control: Towards Innovative Development of Metallic Structural Materials.' The project's objective was to establish an innovative materials design and development framework to significantly enhance the performance of metallic materials. This was achieved by actively exploiting inherent heterogeneities, enabling the simultaneous improvement of multiple properties, a feat challenging to accomplish through conventional methods. Specifically, atomic-scale simulations elucidated the hydrogen embrittlement mechanism at the interface of nanoparticles in aluminum alloys, subsequently guiding the design of particles to mitigate this phenomenon [4,5]. Furthermore, the material design concept was pursued to enhance the surface hardening, friction, and wear properties of nitrided steels through controlled nanocluster formation [6,7]. Additionally, the so-called harmonic structure, characterized by a continuous distribution of strong fine-grained regions and a discrete distribution of ductile coarse-grained regions, was investigated to improve the mechanical properties across various alloy systems compared to their homogeneous counterparts [8,9]. The effectiveness of this microscopic morphology was also demonstrated in the optimal design of duplex microstructures [10].

In parallel to the JST initiative, the 'Center for Hierarchical Materials Design' (CHiMad), sponsored by the National Institute of Standards and Technology, addresses a broader spectrum of advanced organic and inorganic materials, consistent with the process – structure – property – performance reciprocity. Its scope encompasses diverse fields such as self-assembled biomaterials, smart materials for circuit design, organic photovoltaic materials, advanced ceramics, and metal alloys. CHiMad's vision aimed to accelerate materials discovery and commercialization through the design and development of hierarchical methods and materials, thereby enabling the complete integration of computation, experimentation, and databases [11]. Accordingly, this project also focused on controlling the hierarchical heterogeneity inherent in materials. Notably, CHiMad made significant progress in data-driven approaches to accelerate novel material design [12,13]. Within this initiative, a database of heterogeneous microstructures was constructed to aid in the discovery and design. For example, Agrawal et al. [14] utilized machine learning to extract physically meaningful parameters from high-dimensional and highly correlated structural features derived from heterogeneous microstructures for fatigue strength prediction in steels. This allowed for parametric optimization to control heterogeneous microstructures with a smaller set of design variables. Furthermore, pioneering efforts within various use case projects have significantly contributed to imparting innovative properties to diverse materials by strategically leveraging their inherent heterogeneity, exemplified by advances in low-dimensional nanoelectronics [15,16] and organic solar cells [17,18].

Mechanical metamaterials constitute a class of artificial materials defined by the manipulation of heterogeneity at the microscale (rather than the atomic scale), resulting in macroscopic mechanical properties that diverge significantly from those observed in natural materials. The unique properties of these metamaterials are predicated on their specifically designed microstructures (as exemplified in Figure 1), which are often methodically arranged as periodic unit cells or Representative

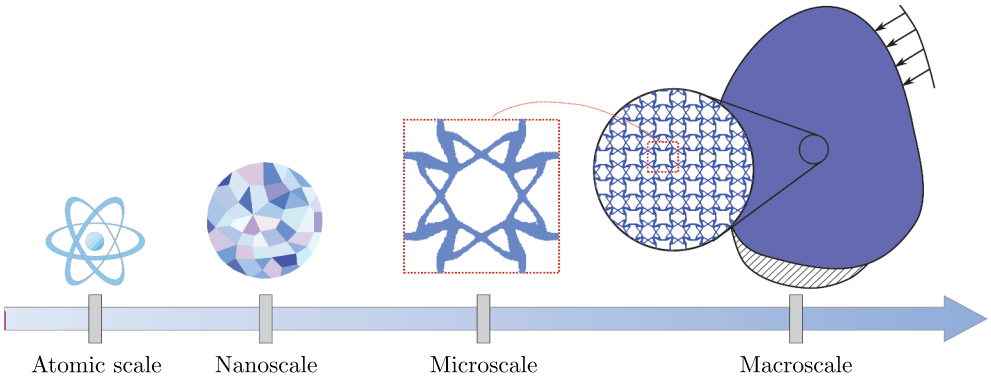

Figure 1. A schematic diagram illustrating how the deliberate manipulation of material geometric features at the microstructural level can induce macroscopic structural properties not typically observed in natural forms. In the context of engineered materials, the underlying microstructure is often conceptualized as periodically arranged unit cells or representative volume elements.

Volume Elements (RVEs) to form the macroscopic material. By manipulating the geometric layouts of these microstructures, macroscopic material properties can be enhanced, frequently surpassing those achievable in natural materials. This capability is not confined solely to mechanical properties; it also encompasses a broad spectrum of phenomena in electromagnetics [19,20] and acoustics [21,22]. Furthermore, the mechanical properties of metamaterials have been shown to develop through complex multiphysics coupling, enabling their fusion with other physical phenomena. The innovative properties of mechanical metamaterials, such as the capacity to exceed the Hashin – Shtrikman (H – S) bounds [23] and exhibit a Negative Poisson's Ratio (NPR) [24–26], have led to diverse applications. These applications span areas such as shock resistance [27], energy absorption [28,29], biomedical engineering [30], and numerous other domains.

While initial efforts in designing mechanical metamaterials relied on empirical knowledge and intuition [31–35], computational approaches grounded in theoretical analysis and numerical simulation have since emerged as the predominant methodology. This computational design framework fundamentally addresses two key questions:

(1) Forward Design: How can macrostructural properties be accurately estimated from a given microstructure's geometric layout?
(2) Inverse Design: How can the microstructure's geometric layout be determined to achieve desired macrostructural properties?

These two queries represent the core challenges in computational microstructure design. However, recent advancements extend beyond these considerations, with emerging efforts addressing a third challenge: optimizing macroscopic structural performance through the strategic arrangement of metamaterials.

The first question (Forward Design) is directly addressed by computational homogenization methods [36–38], which effectively bridge the gap between microscale and macroscale structural properties in multiscale analysis. To address the second question (Inverse Design) – obtaining desired macroscopic material properties – the geometric features of the microstructure are typically explored using various optimization techniques. These include Topology Optimization (TO) [39–43], Deep Learning (DL) methods [44–47], and Genetic Algorithms [48,49], among others. The integration of computational homogenization methods with suitable numerical optimization techniques facilitates the inverse design of microstructures.

Numerous prior reviews [50–56] have extensively explored computational design methods for mechanical metamaterials. However, these reviews have generally focused exclusively on a single methodological stream: either theory-based design methods, represented by TO and prevalent before 2020 [52,56], or data-based methods utilizing AI technology, rapidly developed since the early 2020 s [50,51,53–55]. Consequently, they lack an integrated discussion of both approaches. While a recent review [55] addresses both, it primarily focuses on methodological advances without providing a sufficiently detailed comparative study. Although the scope of this work is confined to microstructures with mechanical properties, the computational design methods discussed are fundamentally generic and widely applicable to general structural and materials design. For instance, Woldseth et al. [57] reviewed both theoretical and data-based methodologies for structural design, focusing on integrating AI technologies within the TO framework. Conversely, in microstructure design, data-driven approaches have evolved into alternative methods to TO, moving beyond mere integration. In light of these developments, this study aims to clarify methodological positions by organizing and comparing both theoretical and data-driven design methods in an integrated manner. Manufacturing considerations introduce another critical dimension. Prior literature, such as Liu et al. [58], has reviewed TO specifically for Additive Manufacturing (AM). The complexity of optimal design solutions derived from TO often necessitates AM, whereas various methods have been proposed to represent geometric features in data-based design. Therefore, we deem it necessary to discuss the connection between computational design and manufacturing from a broad perspective that encompasses not only AM but also other fabrication and processing methods. Furthermore, while some previous studies focus on multiscale design, this review is distinguished by its primary focus on single-unit cell (RVE) design.

Therefore, this study aims to provide readers with a systematic comparative understanding and insight into future perspectives by organizing and analyzing theory-based and data-based design methods for microstructures with mechanical properties in a cross-sectional manner. A common mathematical framework is defined based on design indices, design variables, and computational inverse design methods, providing an integrated structure for organizing both theoretical and data-based techniques. Following this, future prospects are presented through a discussion of the critical connection between proposed microstructure design methods and manufacturing technologies. In this review, we focus on efforts that optimize mechanical properties by exploring the geometric features of single-cell RVE structures. The scope is limited to periodic and deterministic designs, primarily treated under linear and nonlinear elastic assumptions, with an emphasis on associated manufacturing issues. Stochastic or large-scale heterogeneous systems are beyond the present coverage.

The reminder of this paper is organized as follows: Section 2 outlines homogenization methods that establish the link between microstructure heterogeneity and macroscopic material properties. Section 3 presents the formulations and mathematical optimization techniques utilized in the inverse design of mechanical metamaterials, including a comparative discussion using a typical NPR metamaterial design example. Section 4 addresses manufacturing challenges and future prospects related to the geometric manipulation of microstructures that necessitate advanced design techniques. Finally, concluding remarks and a future outlook are presented in Section 5.

2. Computational homogenization approach

This section describes the computational methods for estimating macroscopic material properties from microstructure geometry, specifically utilizing the Finite Element (FE) method for homogenization. This estimation approach is a prerequisite for the inverse design of microstructures tailored to achieve desired mechanical properties. Accordingly, we review these characterization methods and detail their governing equations.

2.1. Estimation of material properties from heterogeneous microstructures

The estimation of material properties from heterogeneous microstructures has consistently been a focal point of research in solid mechanics [59,60]. Analytical approaches to this problem include mean-field theory [61,62] and Eshelby's inclusion theory [63], which provided the foundation for subsequent models such as the Mori-Tanaka model [64] and self-consistent models [65,66]. Complementing these analytical methods are numerical approaches, which encompass the FE method [36–38] and Fast Fourier Transform (FFT)-based techniques [67,68]. Furthermore, numerous mechanical models have been developed to quantitatively characterize the geometric features of heterogeneous microstructures, including image-based modeling [69–71] and microstructure generation techniques [72–74]. This research area has been extensively utilized in the computational evaluation of laminated composites, particularly in the automobile and aerospace industries [75–77].

The computational estimation approaches currently employed in contemporary engineering applications are rooted in mathematical homogenization theory [78,79] (Figure 2). This theoretical approach

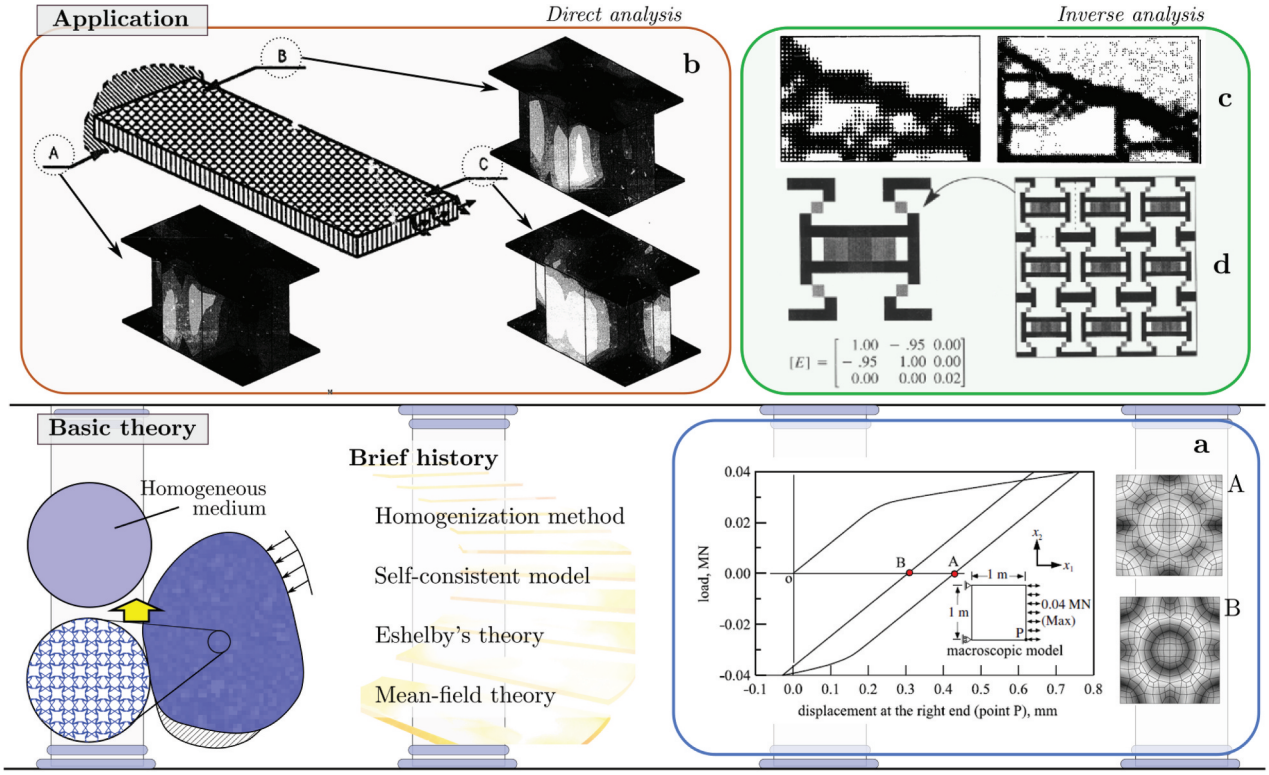

Figure 2. History of the development of theory linking microstructures to mechanical material properties and examples of engineering applications. a. Mechanical characterization of a heterogeneous elastoplastic model subjected to cyclic loading. Darker colors indicate relatively higher von mises stresses [37], copyright 2001, Elsevier. b. Macroscopic stress analysis and local stress distribution diagram for a honeycomb plate. Regions closer to Black represent higher stress [80], copyright 1990, Elsevier. c. Proposal for optimal structural topology design based on homogenization theory, where Black and White correspond to the presence or absence of material, respectively [39], copyright 1988, Elsevier. d. Topology optimization design based on calculating the macroscopic structural properties of microstructures using the homogenization method, in this case for NPR [114], copyright 1994, Elsevier.

is typically discretized and numerically implemented, notably via the FE method, which allows for detailed modeling of microstructure geometry. Such detailed modeling facilitates a quantitative assessment of the microstructure's influence on macroscopic mechanical properties. Consequently, advancements in computer performance and computational algorithms have led to the widespread adoption of homogenization techniques within the engineering domain [80,82]. This capacity to accurately model the geometric properties of arbitrary microstructures has concurrently enabled the exploration of inverse problems, specifically the design of microstructures for desired material properties [83,84]. Moreover, the homogenization method, by characterizing the effective stiffness of macroscopically homogeneous materials and allowing the manipulation of microstructural parameters, has been instrumental in enabling the utilization of shape and topology optimization methods in material design [39,85].

Homogenization methods based on the FE method have evolved into a sophisticated multiscale analysis framework that rigorously links macroscopic constitutive behavior to the microscale mechanics of heterogeneous materials [38,86,87]. In this framework, the boundary value problem of scale coupling between the microscopic and macroscopic scales is derived from mathematical homogenization theory and solved using the FE method. For deformation problems, the scale coupling relationship is typically satisfied by ensuring the correspondence between the macroscopic strain/stress states and the volume-averaged quantities within the microstructure. In particular, the seminal work of Terada et al. [38] integrated two-scale kinematics with a consistent linearization procedure, thereby providing the foundational basis for a general algorithm capable of supporting multiscale analysis of finite deformation problems.

2.2. FE analysis method for periodic microstructure

The RVE is commonly employed as the computational domain for numerically evaluation of macroscopic properties. An RVE is characterized as a microscopic volume element that encapsulates sufficient statistical information regarding the distribution of distinct phases or materials within the microstructure. A periodic microstructural unit satisfying this criterion is often termed a unit cell. For the mechanical assessment of RVEs, a well-established framework for numerical material testing leveraging the FE method is widely implemented in commercial software packages (e.g. Abaqus, ANSYS, Altair OptiStruct, COMSOL Multiphysics). Within this numerical material testing protocol, an FE model of the RVE is constructed and solved for deformation problems under prescribed macroscopic stress or strain states (e.g. a uniaxial stress state pertinent to tensile or compression testing). The application of periodic boundary conditions to the RVE effectively mitigates artificial boundary effects at its periphery. This approach ensures displacement continuity between adjacent unit cells and preserves the mechanical integrity of the composite RVE.

For an RVE in deformation problems, the displacement field $\boldsymbol{w}$ is considered to consist of a macroscopic homogeneous part $\overline{\boldsymbol{u}}$ and a microscopic periodic part $\boldsymbol{u}$. The macroscopic part $\overline{\boldsymbol{u}}$ can be expressed in terms of the macroscopic strain $\bar{\varepsilon}$ and the microscale coordinate $\boldsymbol{Y}$. The total displacement $\boldsymbol{w}$ and the corresponding strain ε can then be formulated as follows:

$$\mathbf{w} = \bar{u} + u = \bar{\epsilon} Y + u \tag{1}$$

$$\varepsilon = \nabla_{\boldsymbol{Y}} \boldsymbol{w} = \bar{\epsilon} + \nabla_{\boldsymbol{Y}} \boldsymbol{u} \tag{2}$$

Consequently, in microscale deformation problems, the unknown field variables are the microscopic periodic displacements $\boldsymbol{u}$. The boundary value problem for the microscopic periodic displacement field $\boldsymbol{u}$ is formulated as follows:

$$\int_{\Omega_{\mathrm{Y}}} \sigma : \nabla_{\boldsymbol{Y}} \eta \, \mathrm{d}\Omega_{\mathrm{Y}} = 0 \quad \forall \eta \in W_{\mathrm{periodic}} \tag{3}$$

where σ represents the stress tensor and Ω_{Y} denotes the volume of the unit cell. η is the variation of the periodic displacement $\boldsymbol{u}$, and W_{periodic} denotes the Sobolev space of periodic functions. Within an RVE, macroscopic variables are defined as the volume average of their corresponding microscale variables, representing the behavior of a homogeneous medium. For example, the macroscopic stress $\overline{\sigma}$ is calculated as follows:

$$\overline{\sigma} = \frac{1}{\Omega_{\mathrm{Y}}} \int_{\Omega_{\mathrm{Y}}} \sigma \, \mathrm{d}\Omega_{\mathrm{Y}} \tag{4}$$

Following these formulations, the macroscopic elastic stiffness tangent tensor $\overline{\mathbb{C}}^{\mathrm{e}}_{ijkl}$ can be calculated by evaluating the macroscopic stress state $\bar{\sigma}_{ij}$ for imposed small strain modes $\bar{\varepsilon}_{kl}$ on an RVE. Based on the components of the resulting $\overline{\mathbb{C}}^{\mathrm{e}}_{ijkl}$, macroscopic material properties such as Poisson's ratio and Zener anisotropic ratio can be obtained [88].

3. Computational microstructure design

In contrast to the preceding section, this section focuses on inverse design methods used to determine the geometric features of microstructures necessary to achieve desired mechanical properties. We specifically examine three fundamental components of computational

design methodologies: evaluation indicators, design variables, and inverse design methods. Subsequently, specific examples of mechanical metamaterials, particularly those exhibiting NPRs, will be presented.

3.1. Interrelationships of design components

We begin by analyzing the interrelationships among these three fundamental components within the computational microstructure design frameworks investigated in this study, as illustrated by the Sankey diagram in Figure 3 [51,88–143]. A designer typically defines an optimization problem based on evaluation indicators and subsequently selects appropriate design variables and inverse design methods to achieve the desired properties. The selection of the inverse design method is particularly critical, as it must balance the inherent difficulty of the design problem (i.e. the challenge of exploring an optimal solution space) with economic factors (i.e. computational cost). Depending on the specific problem, a suitable combination of design variables and inverse design methods may exist, or the applicable inverse design method may be constrained by the required degree of design freedom (i.e. the number and dimensionality of design variables). The subsequent subsections will elaborate on these considerations, consistently referring to Figure 3 for contextual alignment.

3.2. Evaluation indicator

In the computational design of microstructures, quantitative evaluation indicators, derived from mathematical descriptions of desired properties, are essential for defining an objective function in structure optimization problems. These indicators typically encompass elastic properties and various characteristic curves. Table 1 categorizes previous research efforts in this domain, subdividing elastic properties into targets focused on Extreme, Isotropy, Multi-functional, and Manufacturability.

While this section is organized based on the mechanical properties used as design criteria to provide readers with an intuitive classification, it is important to note that many of the underlying computational methods share common inverse design techniques.

3.2.1. Elastic properties

Young's modulus E, often referred to as the elastic modulus, quantifies an object's resistance to deformation under uniaxial tension or compression. This effective value $\bar{E}$ is calculated as the ratio of the

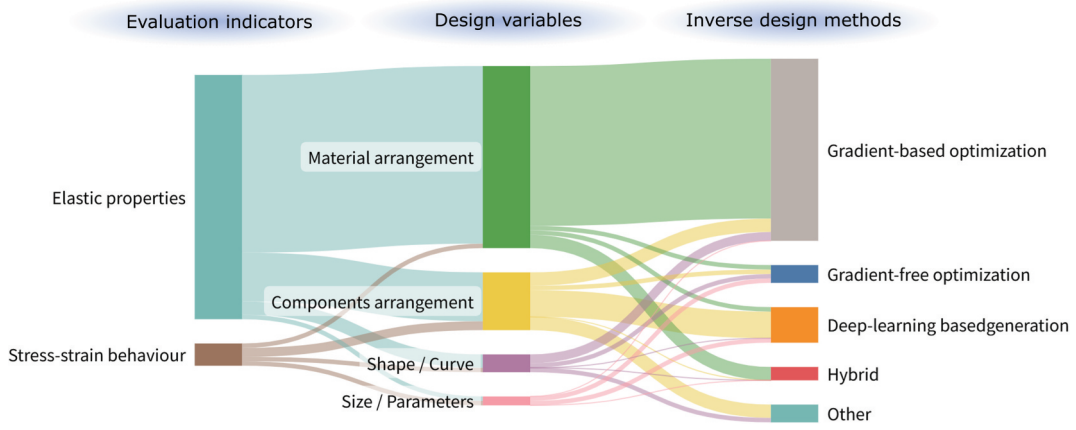

Figure 3. Sankey diagram illustrating the interrelationships among the three main components in computational microstructure design: evaluation indicators, design variables, and inverse design methods [51,81,89–143].

Table 1. Property indicators for computational microstructure design.

Mechanical characteristic		Subclass
Elastic property	Young's modulus	Extreme [51,89–91] Manufacturability [92] Isotropy [93] Multi-functional [94]
	Shear modulus	Extreme [92,95–107] Manufacturability [92] Multi-functional [108]
	Bulk modulus	Extreme [95,97–104,106,107,109–112] Manufacturability [92,113]
	Poisson's ratio	Extreme [88,89,96–99,102–104,107,110–112,114–137] Manufacturability [92]
	Multi-property [138,139]	
Stress – strain relationship	Stress – strain curve [140–143]	

uniaxial stress (tension or compression) to the corresponding strain in the same axial direction. This effective value has shown a strong correlation with the relative density in porous materials as shown in Figure 4. Numerous studies have focused on controlling or exceeding the H– S bounds [23] of the macroscopic effective Young's modulus $\bar{E}$ through microstructure manipulation [51,89–91,93]. For instance, Zhang et al. [90] maximized $\bar{E}$ in both horizontal and vertical directions subject to a given volume constraint. Long et al. [90] achieved an $\bar{E}$ greater than the Voigt estimation or that of conventional materials by exploiting the Poisson effect Figure 4(b). Mao et al. [93] obtained a material distribution for the microstructure that achieves the H – S bounds for isotropic elasticity Figure 4(e), representing a theoretical boundary for evaluating the maximum effective physical property of multiphase materials [23]. Bastek et al. [91] proposed a truss structure with fully tailored anisotropic stiffness. Zheng et al. [51] produced diverse different Voronoi lattices with target relative density and Young's modulus $\bar{E}$ Figure 4(g).

The shear modulus G, also known as the rigidity modulus, measures an object's resistance to deformation under torsion or shear. The effective value $\bar{G}$ is calculated as the ratio of the applied shear stress to the resulting shear strain as shown in Figure 4. Numerous efforts [92,95–108] have aimed to control or achieve the H–S bounds of the macroscopic effective shear modulus $\bar{G}$. Neves et al. [95] and Paulino et al. [96] maximized the effective shear stiffness $\bar{G}$ under given volume constraints, with the latter also achieving near-zero $\bar{G}$ based on a functionally graded material distribution. In contrast, Huang et al. [106] applied BESO (Bidirectional Evolutionary Structural Optimization) to maximize $\bar{G}$ and eliminate ambiguous property values Figure 4(c1). Awrejcewicz et al. [99] investigated the effect of hole placement in the design region as a technical constraint on the optimal solution. Du et al. [105] fabricated and tested a lattice structure inspired by a TO solution to improve the stiffness of a hexagonal lattice structure. Zhang et al. [100] investigated the effect of the initial solution on the optimal outcome. Zhou et al. [108] proposed a mathematical design for multifunctional microstructures with low shear modulus and high thermal conductivity for semiconductor die-bonding layers.

The bulk modulus K is defined as the measure of an object's resistance to volumetric strain when subjected to uniform compression from all directions. The effective value $\bar{K}$ is calculated as the ratio of the applied pressure to the resulting volumetric strain as shown in Figure 4. Computational design efforts utilizing the effective volumetric modulus $\bar{K}$ as a design indicator include the following studies: Gibiansky and Sigmund

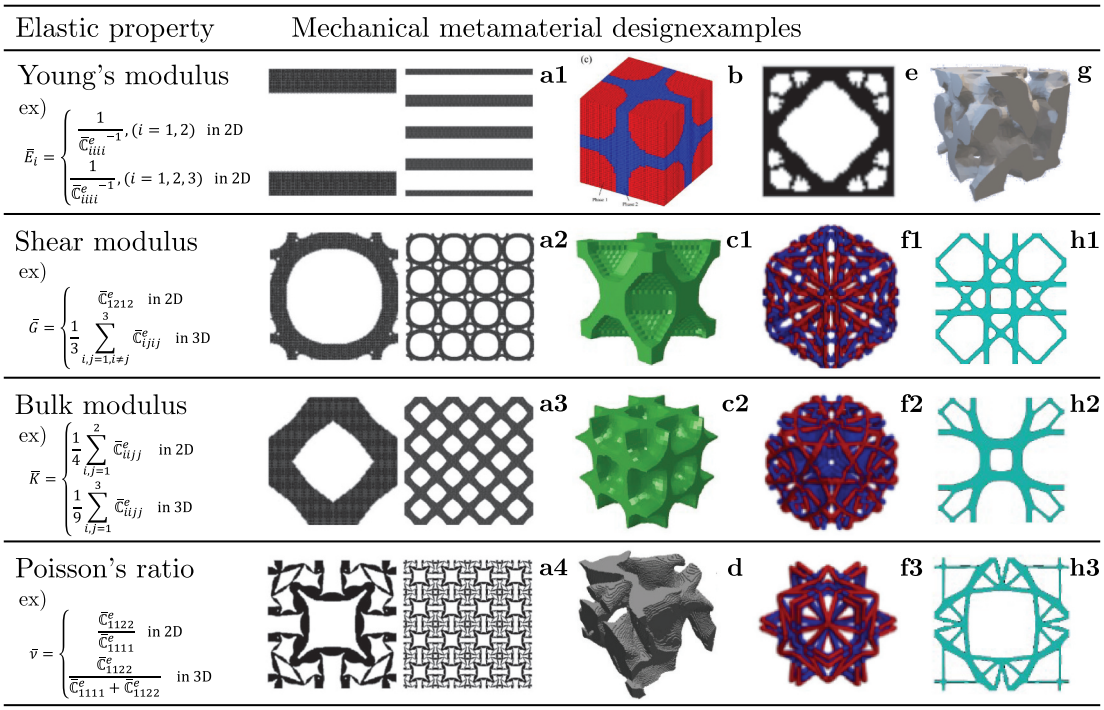

Figure 4. Computational designs of microstructures based on evaluation indicators of elastic properties, including equations for each elastic property [52,90]. a1–a4. Design examples for all elastic properties [97], copyright 2010, John Wiley and Sons. b. Designs exceeding the Young's modulus by leveraging the poisson effect [90], copyright 2016, Elsevier. c1, c2. Designs obtained using beso to eliminate ambiguous property values [106], copyright 2011, Elsevier. d. Design solutions suitable for direct manufacturing without post-processing [92], copyright 2014, Elsevier. e. Design achieving the Hashin–Shtrikman upper limit for isotropic elasticity [93], copyright 2020, Science Advances. f1–f3. Multi-material designs for lattice structures utilizing the geometry projection method [103], copyright 2020, Elsevier. g. Voronoi lattice designs with targeted relative density and Young's modulus [51], copyright 2023, John Wiley and Sons. h1–h3 Robust design considering material uncertainties [103], copyright 2021, Elsevier.

[109] obtained a microstructure design solution with a $\bar{K}$ that exceeds the H– S bounds, employing two different materials and a void. While their effort utilized continuum-based TO, Barbarosie and Toader [110] demonstrated that a similar optimal design solution could be obtained using shape optimization. Takezawa et al. [113] obtained a design solution that maximizes the $\bar{K}$ of a lattice structure, assuming manufacturing by electron-beam melting, while maintaining a sufficiently large hole for metal powder passage.

Poisson's ratio ν is defined as the measure of an object's lateral deformation (shrinkage or expansion) relative to its longitudinal deformation when subjected to uniaxial stress. Its effective value $\bar{\nu}$ is calculated as the ratio of the transverse strain to the longitudinal strain of an object under uniaxial tension as shown in Figure 4. Although Poisson's ratio is commonly considered to range from 0 to 0.5 in natural materials, the computational design of mechanical metamaterials with a NPR was pioneered by Sigmund et al. [114,115]. Subsequently, the development of design methods has been actively pursued, prominently employing TO [89,96–99,110,111,116–122], followed by DL-based approaches [134,136,137,144]. Since continuum-based TO and DL-based design will be analyzed in detail later, only other related efforts are primarily described here. Kazemi et al. [103] proposed a method enabling continuous or discrete placement of multiple materials in a lattice structure using the geometry projection method Figure 4(f3).

Finally, several studies have focused on considering these elastic properties in combination. For example, Ma et al. [138] proposed a shell lattice structure designed to maximize isotropic Young's modulus and bulk modulus, achieving a characteristic value of nearly 80% of the H–S bounds. Additionally, Zheng et al. [131] designed an auxetic metamaterial based on a mathematical definition, which was manufactured in polymer resin and subsequently nickel-coated to improve the low stiffness of auxetic materials. Furthermore, Zeng et al. [139] investigated the gradient distribution of heterogeneity observed in biological organisms and geological formations. They replicated this by distributing the geometrical features of the microstructure in a gradient manner, thereby tailoring its effective elastic property values. This approach yielded gradient mechanical metamaterials, such as porous structures mimicking bone, that achieved the desired mechanical properties for applications like hip joints.

3.2.2. Stress – strain relationship

Compared to the linear elastic properties described previously, considering stress – strain relationship, including nonlinear material responses and instability (such as local buckling), as a design indicator is significantly more challenging. To effectively address this nonlinearity, design variables beyond simple material distribution (as used in standard TO) are frequently employed, as shown in Figure 3. Furthermore, inverse design methods other than gradient-based approaches tend to be favored for designing the stress – strain curve. This preference stems from the inherent difficulty in analytically formulating and evaluating the sensitivity of design variables in highly nonlinear regimes. Although examples remain limited, recent data-driven design utilizing DL has made such complex approaches feasible.

In the following, we introduce efforts to design stress – strain curves based on gradient-free optimization and DL-based generation of heterogeneous microstructures. An approach utilizing a genetic algorithm as a gradient-free method was proposed by Wang et al. [140] Figure 5(b). This computational design approach aimed to achieve a target stress – strain curve by designing a shell-based mechanical metamaterial inspired by Triply Periodic Minimal Surfaces (TPMSs), known for offering high strength and light weight compared to conventional lattice structures. Literature employing DL-based generative design includes [141–143]. Ha et al. [141] and Wei et al. [143] parametrically modeled lattice and hexagonal honeycomb structures, respectively, and generated design solutions using DL to achieve desired stress – strain curves. Notably, the work by Ha et al. [141] also considers the effects of manufacturing errors by including operational verification results through 3D printing Figure 5(a). In contrast, Wang et al. [142] obtained the optimal material distribution for a similar problem by using a TO solution as the training data for DL Figure 5(c). In this context, TO is used to generate reference solutions or training data, effectively serving as a preliminary design or guidance step for DL-based design. The overall design methodology is thus defined as a hybrid combination of gradient-based optimization and DL generation.

3.3. Design variables

Design variables play a critical role in the computational design of microstructures by parameterizing their geometric features. These variables concurrently define the design space in which candidate solutions exist and influence the geometric complexity of the resulting structures. While a larger design space offers greater design freedom, it also entails a higher computational cost for finding the optimal solution. Therefore, the determination of design variables requires careful consideration,

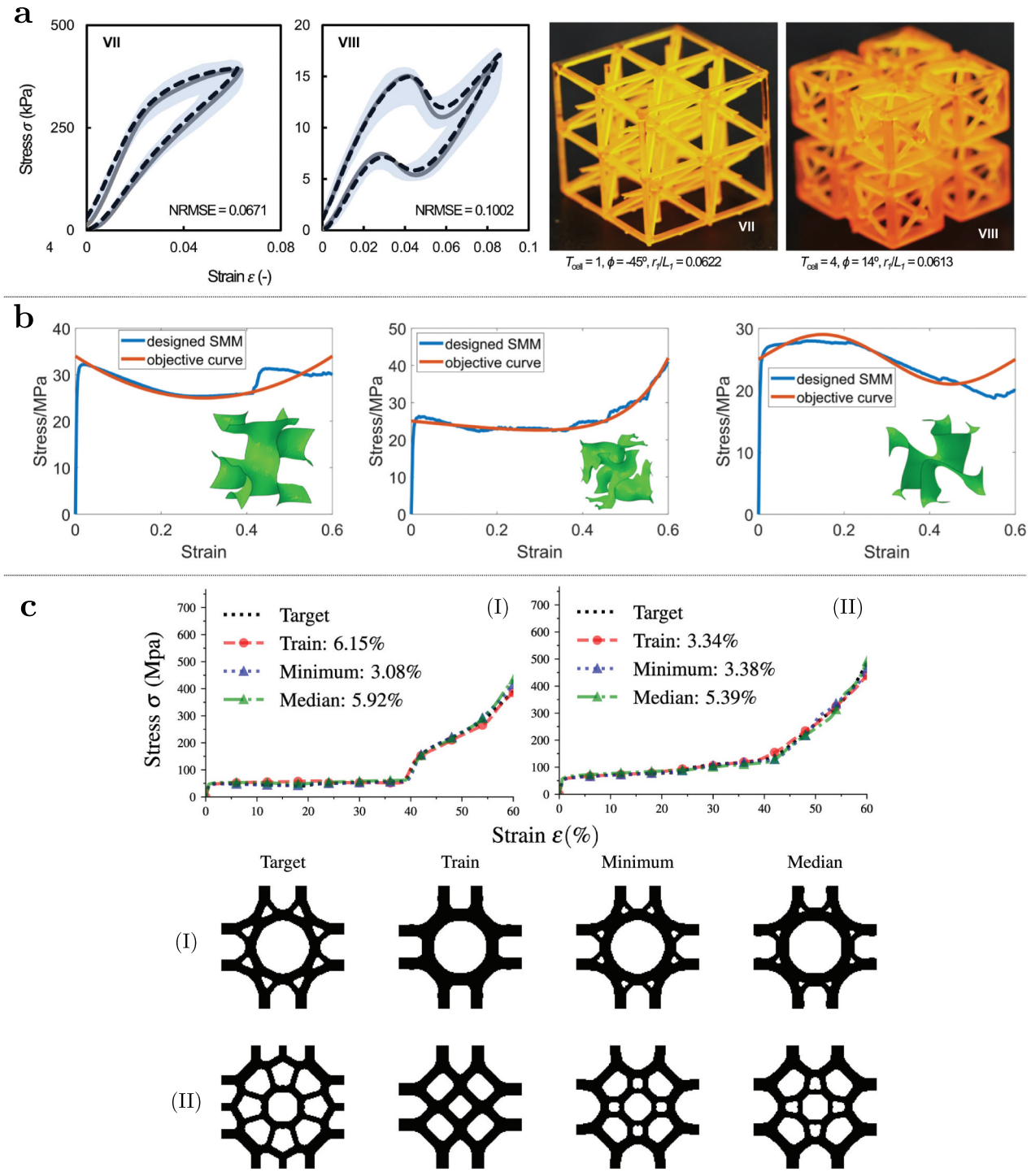

Figure 5. Computational designs of microstructures based on evaluation indicators of characteristic curves: a. Lattice design solution considering process-dependent manufacturing errors [141], copyright 2023, Springer Nature; b. Shell-based mechanical metamaterial concept inspired by TPMSs [140], copyright 2022, Elsevie; c. DiffMat, which utilizes a topology optimization solution as training data for DL [142], copyright 2024, Elsevier.

combining ingenuity with mathematical search or generation methods. In this section, design variables are summarized and reviewed in Table 2, categorized based on material arrangement, member arrangement, shapes and curves, dimensions, and other types.

Computational design efforts are broadly centered on structural optimization methods (classified by updatable geometric features: topology, shape, and size optimization) and DL-based generation. DL-based design allows for a wider variety of design variables because it does not require the analytical derivation of design sensitivity for property updates. Although many DL-based variables offer less design freedom than full material distribution, they can still facilitate changes in microstructure topology. Based on these distinctions, the variables are classified in Table 2 into: material distribution; structural member distribution (as an aggregate with defined geometric

Table 2. Classification of design variables in computational microstructure design.

Structural representation type	Design variables
Material arrangement*	Microscopic volume fraction [95,97]
	Element density [89,92,96,98,99,112,119,142]
	Element density based on NURBS basis function [127,130]
	Level-set function [102,103,116,120,122]
Component arrangement**	Truss's layout [114,115,119,147]
	Lattice's parameters [135,141]
	Voronoi diagram [51,134]
	Slit layout [136]
Shape/Curve (Surface)	Geometric shape boundary [110]
	Shell lattices [138]
	Triply Periodic Minimal Surface (TPMS) functions [131]
	Shell's parameters [140]
Size/Parameters	Honeycomb based cell's parameters [29,143]

*Arrange the presence or absence of material at any location in the design domain; **Arrange the presence or absence of components with some geometric features in the design domain.

characteristics); and shape, size, and defining parameters.

Design variables based on material arrangement offer the highest degree of design freedom in representing microstructural configurations, typically by varying Young's modulus E at arbitrary locations within the RVE. Previously, methods including volume fraction [95], density [92,98], and level-set functions [116] have been used to indicate the presence or absence of material. While volume fraction and density methods suffer from material grayscale (ambiguous material presence), structural representation and update methods based on level-set functions have been proposed [43,145] to avoid such issues. However, level-set based TO is limited by its difficulty in autonomously creating new holes and its strong dependence on the initial design, making flexible topological changes challenging. In both representation methods, the design variable space is inherently high-dimensional. Consequently, the design sensitivity is frequently derived using the adjoint variable method [146], and the optimal solution is explored via gradient methods.

The category of structural component arrangements offers a wide variety of design variables, focusing here on truss layouts, lattice parameters, Voronoi diagrams, and slit layouts. A truss layout represents an arrangement of pin-jointed linear members [114,115,119,147], whereas lattice structures use rigidly joined members, transferring bending moments and allowing for a more continuum-like representation [135,141]. Zheng et al. [51,134] designed microstructures using the Voronoi diagram technique for RVE partitioning based on randomly generated points. Although this yields complex configurations, the direct manipulation of 2D/3D point arrangements offers advantages as a data generator for DL due to its efficiency in preparing diverse candidates. While these methods focus on component placement, Kang et al. [136] focus on the placement of geometric slits within the RVE, noting their ease of fabrication by laser cutting in plate materials.

To represent the shape or curve of a microstructure, methods extend beyond manipulating geometric boundaries at the nodal level [110] to mathematically define the geometry using approaches such as Triply Periodic Minimal Surfaces (TPMSs) [131] and shell-based concepts [138,140]. For instance, Zheng et al. [131] designed an NPR microstructure using TPMSs to represent 3D surfaces. Wang et al. [140] proposed the shell-based mechanical metamaterial concept, also utilizing TPMSs, where the geometry is assigned a thickness as a shell element to maintain a fixed volume fraction within the RVE.

Finally, efforts utilizing structural representations based on size/parameters, which offer the least degrees of design freedom, include [29,143]. Using dimensions and parameters as design variables offers the advantage of enabling a global view of the design space, though the designer must provide an initial design that exhibits some desired properties. Both cited studies manipulated the geometric configuration by representing the re-entrant honeycomb structure with multi-location dimensions based on prior knowledge.

The designer must align the choice of design variables with the size of the design space and the associated computational cost, which ultimately dictates the selection of the inverse design method. Figure 3 illustrates key observations regarding this alignment:

- Material distribution, which creates a vast design space, typically necessitates gradient-based optimization methods to efficiently identify promising solutions through sensitivity analysis.
- Studies using other design variables (component arrangements, shapes/curves, or dimensions), which result in relatively smaller design spaces, allow for greater flexibility in selecting inverse design methods, including empirical search, gradient-free methods, or DL-based generation.

While gradient-based methods offer excellent search efficiency, they often have a limited search range within the design space. Conversely, gradient-

free methods and DL-based generation provide a more global view of the design space. Hybrid methods present a promising computational design approach that combines global search capabilities with flexible structural representation.

In this context, a design method combining TO and DL-based generation was proposed to utilize material distributions as design variables. This approach is particularly effective when controlling the balance of property distributions in a database is important, as TO allows for the generation of samples whose properties closely match target values. However, this TO-based generative method must be recognized as only one strategy. While some methods employ TO to generate samples closely achieving target properties, forward heuristic approaches that generate similarly promising samples also exist [148]. For example, Wang et al. [148] generated data with a wide range of balanced property distributions by simulating microstructures and properties in a forward manner based on a physical model. In any case, TO-based methods represent one effective option for manipulating the balance of property distributions in a database, alongside other inverse design approaches and forward generative strategies.

3.4. Computational inverse design method

Despite the successful determination of evaluation indicators and design variables, obtaining the desired mechanical properties in the mathematical design of microstructures remains challenging. This section outlines the methodologies for identifying optimal design variables, with the objective of optimizing, minimizing, or achieving a target evaluation index. These methods can be broadly categorized into:

- **Iterative inverse analysis**, which employs repeated computation to improve design variables using estimates derived from mechanical constitutive laws.
- **Heuristic approaches**, such as gradient-free optimization (e.g. genetic algorithms mimicking natural selection) or efficient probabilistic methods.
- **Non-iterative inverse generative approaches**, driven by AI-based empirical principles or intuition.

These numerical design methods, which are also applied in general structural optimization, are categorized, and relevant previous research is reviewed and discussed below.

Although some computational design efforts use DL for forward analysis (to compute evaluation indicators for microstructures), this paper focuses exclusively on methods employed for inverse analysis. Thus, inverse design methods used to explore or generate design solutions are categorized in Table 3. The primary classification in Table 3 distinguishes between iterative and non-iterative methods:

- **Iterative Design** is defined as optimization-based inverse design that requires repeated computation to systematically improve the evaluation indicators.
- **Non-Iterative Design** is defined as generative-based inverse design that provides a design solution in a single, one-shot step without such a repeated process.

We note that while a previously cited review [149] adopts a similar classification, we explicitly define these terms to structure our discussion. In recent years, combination (hybrid) methods have also been proposed, where iterative and non-iterative approaches are integrated within a single inverse design process, often applied sequentially, rather than employing one exclusively.

Iterative methods are classified into two categories based on how the design solution is updated: gradient-based and gradient-free methods.

Gradient-based methods involve updating design variables by obtaining design sensitivity, which serves as a guideline for improving the evaluation indicators. This sensitivity is typically obtained through computational analysis, primarily based on the adjoint

Table 3. Classification of computational design methods for microstructures.

Methodology Category		Method and reference
Iterative	Gradient-based optimization	Ground structure [114, 115]
		SIMP [97,98]
		Level-set-based method [116,120]
		Others: BESO [106]; ITO [127]
	Gradient-free optimization	Genetic algorithm [135,140]
		Bayesian [153]/Kriging-based [104] optimization
Non-iterative	Mathematically defined design	Triply Periodic Minimal Surface functions [131]
	Deep generative model	Generative Adversarial Network (GAN) [93]
		Conditional GAN [51,134]
		Variational Auto-Encoder [143]
		Diffusion model [157]
Combined		Topology optimization – Deep neural network [107]
		Topology optimization – GAN [139]
		Topology optimization – Diffusional Model [142]

*Genetic algorithm can be recognized as iterative methods with focusing on updates between generations.

variable method, with respect to the current design solution. TO began approximately 30 years ago with Sigmund's use of truss-like material elements to represent heterogeneity and obtain microstructures with NPR [114,115]. Subsequently, with advancements in computational speed, TO methods have been established for the numerical design of microstructures based on material heterogeneity. Representative TO approaches include efforts utilizing methods such as SIMP (Solid Isotropic Material with Penalization) [97,98] and level-set-based methods [116,120]. Recent developments have broadened the scope of gradient-based inverse design:

- Approaches now leverage automatic differentiation from DL models [150].
- Differentiable simulators enable GPU-based parallelization and acceleration [151,152].

Other developments include the BESO and ITO (Isogeometric Topology Optimization) approaches [106,127], which aim to address the ambiguity of structural boundary representation common in conventional TO methods.

A typical example of a gradient-free method is the empirical design solution search method, represented by a genetic algorithm (GA) that mimics biological evolution. Due to its empirical nature, GA is computationally more expensive than gradient-based methods. Consequently, the design variables used in GA approaches [135,140] often involve the arrangement of members and surfaces with fewer degrees of freedom than material distribution. In contrast, other efforts use Bayesian/Kriging-based optimization methods that efficiently search for optimal solutions by employing estimation (interpolation) models to reduce the number of necessary evaluations. Matthews et al. [153] employed Bayesian optimization to design the geometric features of the microstructure, thereby increasing the probability of obtaining an optimal solution. Liu et al. [104] proposed a gradient-free design method for material distribution by interpolating the design spaces based on a Kriging-based surrogate model.

Non-iterative methods leverage DL for generative design. In this approach, a batch of candidate designs is prepared in advance and evaluated through numerical material testing, and potentially 3D printing and experimentation, to facilitate the learning process. This enables the direct generation of a design solution that achieves the desired evaluation indicators without relying on the iterative improvement information used in optimization. The ability to generate multiple candidate design solutions simultaneously is analogous to conventional iterative design sampling. We focus our discussion on Deep Generative Models (DGMs). DGMs are a subset of DL models that specialize in generative tasks, capable of learning latent probability distributions of data and generating new samples.

Generative Adversarial Networks (GANs) [44], a type of DGM, consist of a generator network and a discriminator network, which have often been used for pseudo-image generation. The generator creates new data from random noise, while the discriminator distinguishes generated data from real data. Through this competitive interaction, the generator gradually becomes capable of producing data closer to real samples. Mao et al. [93] proposed a mathematical design method for microstructures using GANs to achieve target dynamical properties without relying on experience or prior knowledge. While ordinary DGMs learn the entire data distribution and allow extensive exploration of the latent space, conditional DGMs [154] can generate data based on conditions such as labels and performance indicators, offering the advantage of efficiently designing according to target properties in computational design. Using conditional GANs [45], Zheng et al. [51,134] enabled the rapid generation of new microstructure patterns with designer-defined properties. The Variational Autoencoder (VAE) [46] was also used to generate new microstructure patterns across datasets [104], confirming that new patterns beyond the dataset can be readily obtained. Besides GANs and VAEs, the Diffusion model [155] is another representative DGM. In computational design, diffusion model-based methods allow for flexible exploration of a wide design space while maintaining the high quality of the generated microstructures [156].

It is known that a trilemma exists between these three representative DGMs (VAE, GAN, and Diffusion Model), concerning high sample quality, model diversity, and fast sampling [157]. That is, none of the methods can satisfy all three simultaneously: GANs have limited diversity, VAEs tend to produce unclear output design solutions, and the Diffusion model is computationally expensive. Model selection in computational design therefore depends on which aspect of this trilemma is deemed most important for the application.

Both iterative and non-iterative methods possess distinct advantages and disadvantages. For instance, TO (iterative) tends to limit the scope of design searches, yet its sensitivity analysis based on constitutive laws can efficiently and iteratively improve the design solution. In contrast, DGMs (non-iterative) can sample a broad range of the design space but require a substantial amount of data for pre-training, including both promising and unpromising design candidates. In terms of optimizing search coverage and design efficiency, two main hybrid strategies exist to compensate for each other's limitations:

(1) **Preparation of training data**: DGMs are pre-trained using candidate design solution data obtained from TO [107,139,142].
(2) **Post-exploration and refinement**: Initial design space exploration is performed with a DGM, followed by further design improvement using TO.

Furthermore, attempts to effectively use DL in the sensitivity analysis of TO have also been reported [158,159].

3.5. Design examples of Negative Poisson's Ratio metamaterials

The preceding sections reviewed the respective elements of computational microstructure design: evaluation indicators, design variables, and inverse design methods. This section provides a comparative overview of representative computational design methods, focusing specifically on NPR metamaterials. NPR metamaterials are selected for this comparison because their properties are difficult to obtain compared to other elastic properties (as noted by Liang and Piotr [98]), which has stimulated the active development of diverse design methodologies. By analyzing the efficiency and limitations of these methods, we organize their advantages and disadvantages and establish comparative criteria: computational cost, reusability, design pre-processing requirements, and search coverage. Specifically, this comparison will focus on TO, a representative iterative method, and DL generation methods, which exemplify non-iterative approaches.

Figure 6 illustrates the evolution of TO and DL-based design for NPR metamaterials. Efforts utilizing TO [114] commenced in the 1990 s Figure 6(a) and have since expanded to address more advanced design problems, including multi-material design [121] Figure 6(c), nonlinear design [125] Figure 6(d), and designs considering misalignment [88] Figure 6(e). Subsequently, a rapid proliferation of initiatives leveraging data-driven design with DL generation has led to significant advancements [51,136,137] Figure 6 (f-h). Broadly, as noted in the previous section, TO considers continuum-based material distribution, whereas DL generation often focuses on the arrangement of geometrically coherent components. A continuum-based DL design was notably implemented within a hybrid TO and DL-based design framework [107] Figure 6(i).

The characteristics of both design methods are compared based on computational cost, design method reusability, design pre-processing requirements, and search coverage in the design space (Table 4). From a computational cost perspective,

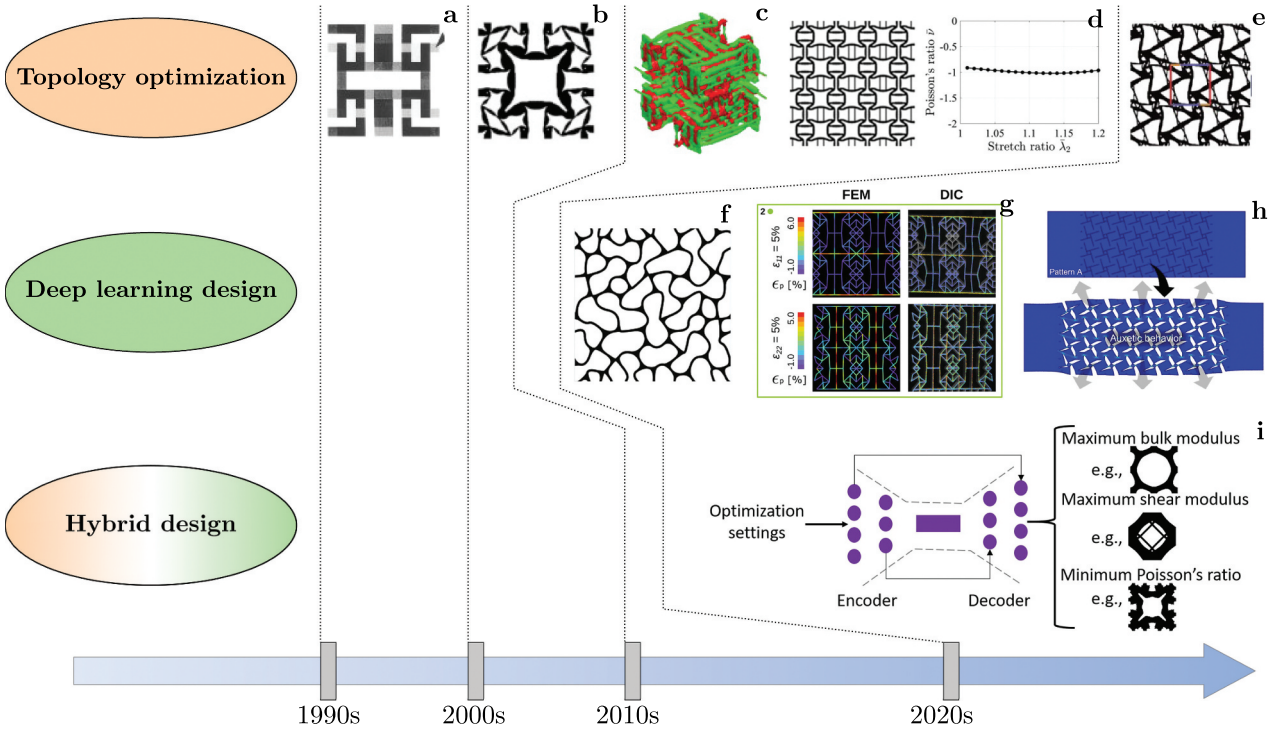

Figure 6. Research history of inverse designs for NPR metamaterials. a. First application of topology optimization to an NPR design problem [114], copyright 1994, Elsevier; b. Established NPR topology optimization design [97], copyright 2010, John Wiley and Sons; c. Example of design based on 3D multi-materials [121], copyright 2017, Elsevier; d. Consideration of nonlinear response [125], copyright 2019, Elsevier; e. Design incorporating misaligned periodic boundary conditions [88], copyright 2025, Elsevier; f. Structural representation using Voronoi diagrams [51], copyright 2023, John Wiley and Sons; g. Size-agnostic inverse design of random-network mechanical metamaterials [137], copyright 2023, John Wiley and Sons; h. Design utilizing slit placement as a variable alongside operational verification [136], copyright 2024, Elsevier; i. DL-based design achieved via pre-training with topology optimization [107], copyright 2020, Elsevier.

Table 4. Comparison of topology optimization and deep learning-based design methods for NPR metamaterials.

	Topology optimization	Deep generative model
Computational cost	Design decision: Slow Overall: Problem-dependent	Design decision: Rapid
Reusability	Tuning required	Easy
Design pre-processing	Sensitivity analysis	Generate training data
Search coverage	Local with sensitivity	Global

*: From determining the desired mechanical properties to obtaining the geometric features of the microstructure; **: From design method development to obtaining microstructural design solutions.

DL-based design is rapid and superior for determining individual design solutions; however, its overall computational efficiency across the entire design process is problem-dependent due to substantial initial training costs. Conversely, TO generally requires a new optimization process for every design target, as it begins from scratch in each run. TO identifies the optimal microstructure by sequentially updating the design candidate from an initial or tentative solution based on design sensitivity derived from physical laws. Because it is a sequential, gradient-based method, TO primarily performs a local search. This search is highly efficient due to its physical guidance but consequently lacks global search coverage. In contrast, DL-based design offers a global view of the design space, but this comes at the cost of requiring the model to learn a large number of unpromising design solutions, making the initial training phase computationally expensive. The key advantage of DL is that once trained for the mechanical properties of interest, it can respond rapidly to changes in desired properties and leverage accumulated training data over time, making it highly reusable and extensible.

Both methods have distinct limitations and practical requirements:

- Topology optimization is constrained by the need to restart optimization for each new design target and its primarily local search nature.
- Deep learning-based design is dependent on large, high-quality training datasets and may perform poorly for designs falling outside the training domain.

Regarding practical requirements, TO generally demands guidelines for obtaining desirable design solutions through physics-based sensitivity analysis, while DL requires extensive data preparation and substantial computational resources for training. These two methods also find application in different contexts:

- Topology optimization is best used to find a design solution for a novel, pioneering property that is not yet known and for which no data is available.
- Deep learning is best used to find a design solution in real time when there are plenty of existing examples of the design target, when the design target can easily be generated, and when the design target is dynamically and iteratively changing.

3.6. Discussion on open challenges

The previous section organized and comparatively analyzed prior efforts in the computational design of microstructures across key elements. This included a comparison between the theory-based TO approach and the data-driven DGM approach, with reference to NPR characteristics. While presenting an overview of the latest advances, several significant challenges remain in realizing target properties based on these computational design methods. This section focuses specifically on these unresolved issues, organizing the theoretical and implementation bottlenecks. Note that manufacturability, one of these key challenges, will be discussed separately in Future perspectives for the manufacturing.

3.6.1. Tackling one-to-many mapping problem

In inverse design, a one-to-many mapping fundamentally exists, meaning multiple distinct design solutions can correspond to a single target property. This stems from the inherent non-uniqueness of inverse problems. This non-uniqueness has posed a significant challenge in data-driven computational design: traditional regression models, based on a one-to-one correspondence, cannot represent multiple solutions, leading to forecasting ambiguity and instability in solution exploration while aiming to safeguard design freedom and diversity. To address this, conditional generative models, such as conditional GANs and conditional VAEs, have been applied to inverse materials design. Unlike conventional artificial neural networks, conditional DGMs can probabilistically generate a set of candidate designs conditioned on the target properties [154]. This capability enables the efficient exploration and generation of physically plausible and diverse design candidates, thereby practically mitigating the non-uniqueness problem inherent in inverse design.

3.6.2. Generation of novelty

Future computational design endeavors will increasingly necessitate the generation of novel microstructures. Achieving this requires simultaneous progress in two critical areas: the establishment of robust evaluation indicators and the advancement of inverse design methods. The former demands the development of diverse evaluation indicators, extending to metrics for multi-objective, multi-physics, and intelligent metamaterials [51,53,56]. The latter involves innovative efforts, such as creating the evaluation indicators themselves to drive the generation of entirely new materials.

As discussed previously, while TO excels at exploring unknown design solutions, data-based DGMs currently find generating truly novel data challenging. Within this context, efforts are being made to model creativity itself to advance computational design methods beyond human intelligence [160]. For example, the Creative Adversarial Network (CAN) [161] was proposed. It is anticipated that such techniques will be extended to the design of material microstructures in the near future.

3.6.3. Faster and more efficient computation

The design of material microstructures is an inherently complex problem, and the demand for novelty and innovation is likely to increase further. A potential bottleneck in this scenario is excessive computational cost, necessitating ever-greater efficiency and acceleration. The total computational cost required throughout the entire design process is governed by two factors: the fidelity of the performance evaluation and the number of design trials (or the amount of data required).

The fidelity of performance evaluation directly affects the actual performance of the final design solution. From the perspective of computational acceleration, the challenge lies in reducing computational cost without compromising fidelity. A representative approach is the development of surrogate models [160]. Surrogate models aim to achieve low-cost performance evaluation by approximating expensive numerical computation results based on a limited amount of data. However, a known weakness is the deterioration of approximation accuracy in regions where training data is sparse or heterogeneous. A promising solution to this is multifidelity modeling. This technique reduces computational cost by employing evaluations from low-fidelity models to compensate for the reduced number of high-cost (i.e. high-fidelity) performance assessments. Multifidelity modeling is increasingly utilized in the design of material microstructures with specific mechanical properties [162,163].

Secondly, in theory-based computational design methodologies, considerable effort has been devoted to developing techniques that explore promising solutions while minimizing the number of required trials. Conversely, in data-driven computational design methods, the insufficient size of the required datasets has become a major bottleneck.

Future research will require not only the dissemination of data by individual research groups but also the promotion of policies by journal editors and reviewers mandating authors to upload data to centralized databases, as suggested by Bonfanti et al. [55]. Moreover, it is critical not only to construct large datasets but also to ensure data diversity. In inverse design, the data must cover the design space as uniformly as possible. This likely necessitates diversifying (i.e. universalizing) the design variables that are currently often limited to specific initiatives, though collecting such diverse data entails high costs. Addressing these challenges, Zheng et al., in their future outlook, proposed that the application of quantum machine learning and large-scale language models could accelerate the construction of diverse and large-scale datasets [51]. This led them to subsequently propose a method that actually utilizes large-scale language models [144].

4. Manufacturing designed microstructure

In this section, we review the practical processes required to realize microstructures obtained through computational design, focusing specifically on manufacturing methods. We first review past research addressing these manufacturing issues, followed by a discussion of future prospects. Note that while computational design methods for multiscale and multiphysics problems share some similarities with the methods discussed here, this discussion is limited to microstructures with mechanical properties due to constraints on scope and space.

4.1. Prototyping of microstructural design solutions

To obtain desired mechanical properties, complex microstructures must be manufactured with high fidelity. Such manufacturing necessitates precision processing tailored to the curvature and fineness of the microstructure, often limiting applicable methods to specialized equipment and advanced technologies. However, the remarkable development of AM technology has led to the emergence of relatively inexpensive 3D printers accessible at the laboratory level. While these 3D printers are generally unsuitable for large-part manufacturing or mass production, they are increasingly capable of prototyping to verify the performance of mathematical design solutions. This

ability to fabricate and verify material behavior is valuable not only for understanding microstructure performance but also for the mathematical design of process-oriented microstructures. This section reviews prior research concerning the manufacturing of mathematically designed solutions.

Studies conducting manufacturing and operational verification primarily employ subtractive and AM techniques. For subtractive processes, methods such as wire-saw cutting [105] and laser cutting [94,136] are commonly utilized. While these techniques enable high-precision processing, their shaping capabilities are limited compared to AM. Conversely, AM facilitates the fabrication of complex structural configurations. Techniques include SLS (Selective Laser Sintering) [92], SLA (Stereolit-hography Apparatus) [89,123,128,134,141], DIW (Direct Ink Writing) [164], EBM (Electron Beam Melting) [113,117], and WAAM (Wire Arc Additive Manufacturing) [165,166]. The proliferation of low-cost desktop 3D printers using SLA, in particular, has made 3D printing an effective tool for rapid prototyping and laboratory-level validation. Furthermore, 3D printing contributes to the generation of data incorporating manufacturing processes. For instance, Ha et al. [141] generated data including process-dependent manufacturing errors to acquire highly accurate performance validation.

While AM facilitates the fabrication of complex geometries, manufacturing arbitrary design solutions remains challenging due to unique process limitations stemming from the printing method and materials employed. Computational design addresses these manufacturing challenges through two main approaches: process-level control and the imposition of geometric constraints.

Process-level control involves either eliminating the need for certain manufacturing processes or actively controlling process parameters to mitigate defects. Andreassen et al. [92] proposed a design method that eliminates the post-processing necessitated by grayscale representations in conventional TO, thereby reducing performance loss attributed to such steps. Several computational design methods explicitly consider AM limitations. Miki et al. [167] developed a TO method to reduce warpage caused by thermal distortion. Yamada et al. [168] developed a method to eliminate closed cavities, and Tajima et al. [169] incorporated overhang constraints. Notably, Takezawa et al. [170] proposed a mathematical design method that integrates process and structure in metal AM by simultaneously optimizing the laser hatching orientation (a process parameter) and lattice density (a structural parameter).

Imposing geometric constraints involves setting geometric constraints (e.g. on hole size and overhangs) on the optimal design solution to ensure fabricability. Du et al. [105] reduced manufacturing complexity by identifying a microstructural configuration with equivalent mechanical properties but limited design freedom within the TO solution. Similarly, Wang et al. [123] achieved equivalent mechanical performance with a simpler structure by performing shape optimization with restricted design degrees of freedom subsequent to TO. Takezawa et al. [113] conducted a computational design of the microstructure assuming EBM fabrication, explicitly ensuring that holes were sufficiently large to facilitate material powder removal during the manufacturing process.

Another important aspect of ensuring manufacturability is the definition of design variables. Since design variables determine the design space and the geometric characteristics of the resulting microstructure, defining them with manufacturability in mind is a key measure to avoid design solutions that are difficult to manufacture. The efforts of Du et al. [106] and Wang et al. [123] (discussed above) can be viewed as examples of this approach. Furthermore, Kang et al. [136] proposed a pattern structure that is easily fabricated via laser cutting of a flat plate, expressing geometric features through the arrangement of slits rather than conventional material distribution. The definition of design variables is thus a critical factor linking numerical design solutions with actual manufacturability.

Finally, it is essential to explicitly incorporate manufacturing uncertainties into mathematical design. Design methods such as [103,119,122,133] have been proposed to account for variations in material properties or shape deviation uncertainties due to the manufacturing process. Ha et al. [141] quantitatively evaluated the uncertainty in the stress – strain relationship caused by resolution and defects in 3D printing by acquiring extensive experimental data, explicitly reflecting these results in the design. These efforts emphasize a shift from an idealized approach to a design based on manufacturing robustness. This establishes a new guideline: the design solution, even if obtained assuming an ideal state in simulation, must be robust enough to maintain the desired performance in a real environment after manufacturing.

4.2. Future perspectives for the manufacturing

The key to addressing the challenge of manufacturing microstructures with specific mechanical properties will be the co-evolution of computational design and manufacturing technology. From structural and process viewpoints, three potential strategic solutions exist for this manufacturing challenge:

(1) **Design Adaptation**: Developing computational microstructural design methods while maintaining current manufacturing constraints.
(2) **Process Advancement**: Advancing manufacturing technology to allow the fabrication of

arbitrary microstructures while utilizing existing design methods.

(3) **Integrated Co-development**: Integrating and co-developing microstructure design and manufacturing processes.

The first strategy involves improving microstructure design by directly incorporating the constraints of assumed manufacturing technology (e.g. minimum machinable dimensions and overhang constraints) into the design formulation. The second strategy is to advance precision microfabrication techniques to enable the manufacture of arbitrary microstructures. Following a discussion of these two interactive approaches, we will focus on the third approach: integrated process – structure – property – performance design.

As previously stated, several computational design methods already integrate AM constraints [167–170], as it has become a mainstream fabrication technology for microstructures. For instance, one notable approach simultaneously optimized the laser hatching orientation (a process parameter) and lattice density (a structural parameter) to integrate process and structure in metal AM [170]. These efforts demonstrate the application of computational design to generate microstructures with desired mechanical properties while actively satisfying manufacturing constraints. Concurrently, advancements in AM technology have been substantial. Literature documents the feasibility of fabricating microstructures at the nanometer to micrometer scale [171]. Recently, high-resolution 3D printing, such as technology using roll-to-roll continuous liquid interface manufacturing [172,173], has enabled the mass production of microstructures with micrometer-scale geometric features. The computational design methods and manufacturing techniques will continue to develop through this strong interaction.

The current co-evolution of TO and AM, however, lacks scalability, making the mass production of mechanical microstructures challenging. This limitation is particularly acute for mechanical metamaterials. Unlike electromagnetic or acoustic metamaterials, whose structural scale is fixed by the manipulated wavelength, mechanical metamaterials exhibit scale-invariant performance (their behavior remains qualitatively similar across different scales given consistent geometry). Applications in architecture, mobility, and soft robotics may demand large-volume manufacturing ranging from a few millimeters to several meters. Therefore, the future necessitates the co-evolution of scalable and mass-producible processes alongside computational design methods rooted in these processes. A promising avenue to address this challenge is an integrated optimization method rooted in multiscale simulation. By simultaneously optimizing manufacturing process conditions and microstructure design, it is anticipated that both performance and manufacturability can be achieved at scale.

An alternative to sophisticated fabrication is the approach of component assembly, which circumvents the difficulties associated with manufacturing complex monolithic geometric features. In this context, intricate RVEs have been decomposed into modularized parts (akin to Lego bricks) to facilitate assembly-based manufacturing while preserving the flexibility of structural representation [174]. The components and their assembly methods, integral to the manufacturing process, can be more directly and intuitively connected to the design variables that define the assembled RVEs. Consequently, computational design that integrates the manufacturing process and structure becomes more straightforward. Computational design methods for this purpose are expected to develop actively. Indeed, a spring-based mechanical metamaterial combining spherical nodes and spring elements has been proposed, and its computational microscopic structural design is constructed by combining multiscale analysis with an inverse design method [175]. Further development of an integrated process – structure – property – performance computational design method that explicitly considers assembly strategies is anticipated. The advantages of such assembled mechanical metamaterials, including their ease of parallel manufacturing and repair, make them highly suitable for applications in architecture, soft robotics, and mobility. Furthermore, these metamaterials may co-evolve with the mass production capabilities of nanometer to micrometer 3D printing technology [172,173] to drive the realization of truly scalable mechanical metamaterials.

5. Conclusion and future perspectives

This review paper aimed to offer researchers and engineers comprehensive insights into the development of design methods by systematically reviewing the inverse design of microstructures with mechanical properties through various computational methodologies.

We first described the homogenization method, a widely used numerical technique, outlining its theoretical background for the forward problem (deriving macroscopic properties from a given microstructure). Subsequently, we focused on the inverse design problem, which aims to determine the geometrical features of a microstructure to achieve desired characteristics. This inverse design landscape was systematically organized by focusing on three basic components: evaluation indicators, design variables, and inverse design methods. Research trends for each

component were discussed, and their interrelationships were visually presented and comprehensively analyzed using Sankey diagrams.

Using Negative Poisson's Ratio (NPR) metamaterials as an example, we compared the theory-based topology optimization (TO) approach with data-driven Deep Generative Models (DGMs). Our comparative analysis revealed their distinct advantages and limitations, showing that their suitability depends heavily on design objectives:

- Topology optimization is preferable for novel problems with limited data or when the evaluation cost is prohibitively high.
- Deep generative models are advantageous when relevant data are available, evaluations are inexpensive, or design reusability is paramount.

These insights extend beyond NPR to complex areas such as nonlinear regimes, multiscale problems, and multifunctional targets. TO is expected to be effective in costly nonlinear or multiscale evaluations, whereas DGM is better suited to multifunctional designs that require rapid screening of the Pareto frontier. Ultimately, hybrid frameworks that integrate the strengths of TO and DGM will be critical for advancing computational microstructure design. While these methods enable effective microstructural design, their manufacturing still presents numerous challenges. We reviewed computational design and advanced manufacturing techniques that address these issues, then presented a strategy for addressing manufacturing challenges in microstructural design with consideration of mechanical performance.

In light of these findings, future research should integrate theory-based and data-driven design methods within a combined framework, thereby complementarily overcoming their respective limitations. Furthermore, from a manufacturability perspective, there remains a critical need to develop computational design methods that account for process-level control and geometric constraints. In this context, the advancement of manufacturing techniques is likely to co-evolve with mathematical design methods. Current challenges also include addressing the inherent one-to-many mapping problem and developing the capability for generating true novelty. Here, computational cost poses a significant bottleneck, with the preparation of large-scale, diverse datasets, the huge computational resources required for learning and optimization, and constraints to ensure manufacturability remaining major obstacles. To overcome these, it is essential to further enhance the synergy between computational design, data-driven modeling, and advanced manufacturing technologies. Beyond computational design methodologies based purely on combining theory and data, the integration of computational, data, and manufacturing technologies holds promise for creating more robust and resilient Digital Twins of manufacturing processes. This approach has the potential to accelerate the implementation of design solutions that combine functionality and practicality, consequently breaking down boundaries hindering industrial application.

Digital technology has evolved to augment, and in some cases replace, not only experimentation but also human decision-making, knowledge, and experience. Computational and generative design represent efforts to mathematically and automatically reconstruct the act of 'design,' which has historically been performed by humans based on intuition, experience, or physical constitutive laws. However, regardless of this progress, it remains the role of humans to establish the foundational framework and define the design problem itself. In fact, the concept of 'design the design process' has been discussed in the context of meta-design and design automation [176,177], emphasizing that how design methodologies themselves are created and adapted by humans will remain important. Based on this perspective, the 'Design of Design' will become increasingly vital in the future. Soon, meta-design approaches that inversely design these computational design methods and generate optimal design methodologies will also be envisioned. The era of design for design automation is rapidly approaching.

Author contributions

CRediT:**Keita Kambayashi**: Conceptualization, Formal analysis, Investigation, Visualization, Writing – original draft Preparation, Writing – review & editing; **Ikumu Watanabe**: Conceptualization, Investigation, Project administration, Supervision, Writing – original draft Preparation, Writing – review & editing.

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