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Multi-material additive manufacturing: a computational design perspective

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ABSTRACT

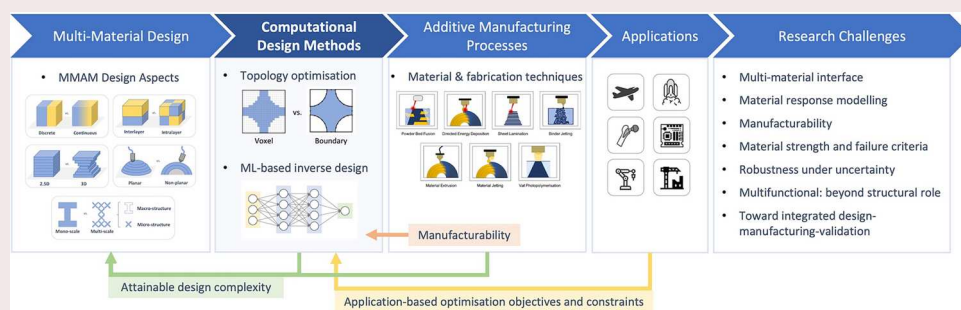
Multi-material additive manufacturing (MMAM) unlocks unprecedented opportunities in engineering, afforded by material and geometric complexity. However, leveraging its full potential necessitates advanced computational design tools tailored to specific application needs and fabrication techniques capable of translating digital designs into physical products with minimal discrepancy. This review provides a comprehensive evaluation of computational algorithms available for multi-material design, encompassing numerical methods like topology optimisation as well as data-driven inverse design strategies. MMAM techniques are evaluated for their multi-material design capability and manufacturing constraints. Key challenges in MMAM design are identified, including multi-material interface, advanced material response modelling, manufacturability, failure constraints, robustness, multifunctionality, and integrated design-manufacturing-validation workflow. Recommendations are made for incorporating these considerations into the optimisation framework. Future research directions are also suggested to pave the way for innovative multi-material applications.

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Multi-material additive manufacturing; topology optimisation; inverse design



1. Introduction

Additive manufacturing (AM) has transformed fabrication by enabling the creation of complex geometric features and customised designs whilst reducing material waste. Building on these advantages, multi-material additive manufacturing (MMAM) expands the possibilities by integrating two or more materials with distinct properties within a single structure. This is particularly advantageous for multi-functional engineering applications across sectors such as aerospace [1] and biomedical [2,3], where certain constraints or competing objectives cannot be met by altering topological/geometric features alone. Currently, MMAM enables a variety of material combinations, such as metals and polymers, with ongoing developments in composites and hybrid materials.

The design space of AM ranges from pre-build, process and post-processing in a broad definition [4]. In this article,

‘design’ refers specifically to part design in the pre-build stage. The selection of feedstock material and process parameters, however, fall outside the scope. The concept of ‘multi-material’ refers to the heterogeneous spatial distribution of at least two solid material candidates across the part at the macro-scale level. Alloys consist of distinct phases but with spatial homogeneity are not multi-material in this context. Figure 1 illustrates five fundamental design aspects of MMAM, in which different combinations allow the generation of diverse designs.

The following concepts are unique to the multi-material context:

- *Discrete vs. Continuous*: discrete refers to the existence of distinct material boundaries at the macroscopic level, while continuous or graded composition leads to smooth material transition

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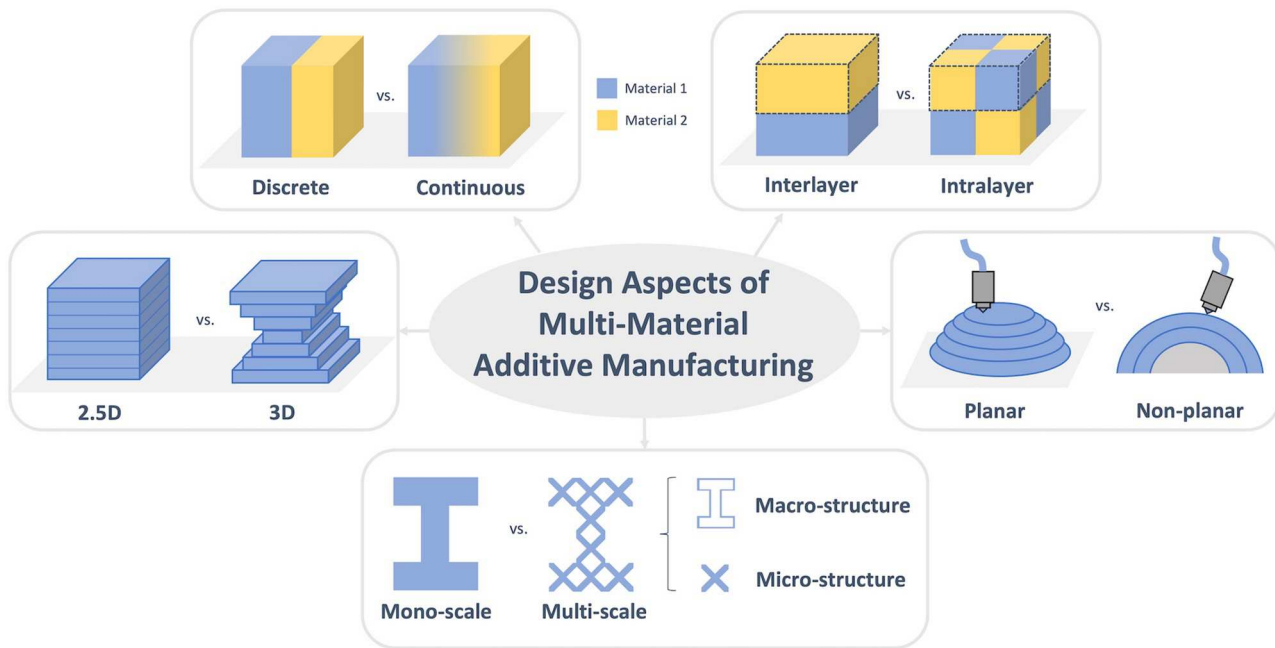


Figure 1. Five fundamental design aspects of multi-material additive manufacturing.

- *Interlayer vs. Intralayer*: interlayer restricts material to alter across layers only, while intralayer allows multiple materials to be present within one layer

The following aspects are general to AM:

- *2D/2.5D vs. 3D*: A 2.5D part involves the uniform extrusion of a 2D design along one direction (typically the building direction), meaning there is no geometric or material variation along that axis. Whereas a 3D design allows for changes in both geometry and material across all three spatial dimensions.
- *Planar vs. Non-planar*: whether the printing layer is a flat or non-flat (i.e. with curvatures) surface
- *Mono-scale vs. Multi-scale*: designs with a single feature scale versus those combining multiple scales, such as macroscopic structures with microscopic unit cells, which not necessarily correspond to physical length scales.

The field of MMAM has garnered increasing research attention over the past five years, with a strong emphasis on fabrication processes and experimental studies. Comprehensive reviews on MMAM were generally categorised by material choices and manufacturing techniques [5–7], while complimentary sections may include post-processing methods, applications, and functional grading capability [8–10]. In the domain of metal MMAM, powder bed fusion (PBF) has been extensively studied [11–17] compared to directed energy deposition (DED) [18]. These works often

highlight specific research challenges related to the process, such as interface characterisation, powder delivery systems, cross-contamination, and simulating melt-pool behaviour, etc. For polymers, Shaukat et al. [19] reviewed material chemistries involved in multi-material vat photopolymerisation (VP), while Patpatiya et al. [20] examined PolyJet 3D printing of fibre-reinforced and functionally graded structures. García-Collado et al. [21] covered polymer-based MMAM in general, remarking on properties, process parameters and applications in addition to technological developments of the fabrication processes. Overall, material – and process-related advancements have been thoroughly summarised. However, critical examination of MMAM techniques offering the promised design flexibility is yet to be undertaken. Maturation of computational design tools should account for process-specific constraints, ensuring advancements in MMAM.

Technical works related to MMAM design are remarked within a broader review topic, such as optimisation for multi-scale lattices [22], data-driven metamaterial design [23,24], machine-learning-assisted topology optimisation (TO) [25,26], and the application of machine learning (ML) in AM [27,28], but the coverage is very limited. To highlight those focusing on multi-material, Esfarjani et al. [29] reviewed TO of additive-manufactured lattice metamaterials, particularly emphasising multi-material types. Choi et al. [30] examined the application of ML in the design and manufacturing of responsive composites through 4D printing. However,

a unified review is required to fairly compare traditional numerical methods and emerging data-driven approaches, which are the two main directions being investigated currently within the structural design community. It is also essential to identify key research challenges causing design-to-manufacturing deviations and to analyse how various design methods address these challenges.

To address the research gap in design for multi-material additive manufacturing (DfMMAM), this article presents a framework that links multi-material design aspects, computational optimisation algorithms, and manufacturing techniques together. First, five fundamental design aspects of MMAM are introduced, demonstrating how their combinations enable diverse design possibilities. Subsequently, Section 2 provides a comprehensive review of existing computational design tools, bridging numerical methods with data-driven approaches. It not only covers methodology development for diverse multi-material design representations, but also application of these methods across design scenarios, and numerical examples for benchmark comparison. An overview to manufacturing techniques, emphasising the required system modifications for multi-material fabrication and their capability to fulfil the defined design aspects can be seen in Section 3. Multi-material applications are examined in Section 4, illustrating different motivations for adopting multi-material solutions across sectors. Research challenges are outlined in Section 5, followed by concluding remarks and suggested future works in Section 6. Overall, this article offers actionable guidelines for

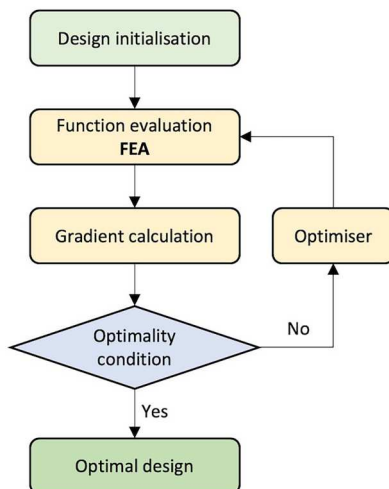
selecting computational tools and manufacturing techniques to leverage multi-material designs for demanding engineering applications.

2. Computational design methods

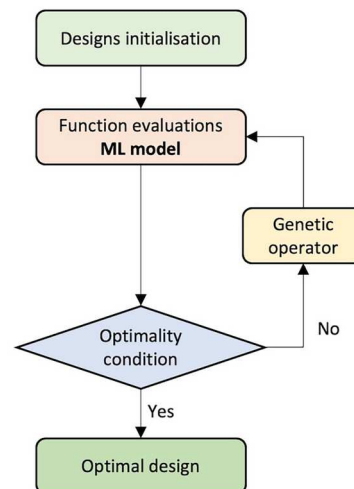
Initial explorations highlighted the potential of multi-material structures, motivating the development of mathematically rigorous optimisation methods to leverage the design freedom afforded. Design variations range from the spatial distribution of materials [31–33], adjusting material mixture ratio [34–36], and testing different material combinations [37,38]. Strategies such as varying geometric parameters [39] and the inclusion of multiple unit cell types [40,41] have also been tested in multi-material lattice structures. Given the varying maturity of MMAM techniques, most studies used polymer samples fabricated via jetting or extrusion, with limited metal samples from PBF. However, empirical approaches are resource-intensive, lack scalability and physical insight, leading to a shift toward computational design optimisation.

Like a single-material design problem, a multi-material optimisation problem can be formulated using design variables, objectives, and constraints. Wherein, the design could be characterised either by volumetric discretisation (i.e. pixel/voxel) or boundary representation. Objectives could be set as maximising/minimising or matching certain performance metrics. Constraints may relate to the bound of material usage, minimum feature size due to manufacturing resolution,

(a) Gradient-Based Method



(b) Indirect Inverse Design



(c) Direct Inverse Design

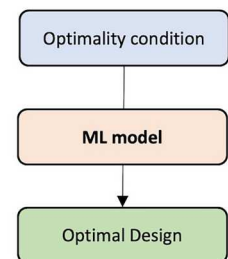


Figure 2. Optimisation workflow in (a) gradient-based method that relies on finite element analysis and sensitivity calculation. (b) indirect inverse design, in which multiple design evaluations will be conducted by the predictive ML models followed by genetic operators to sample new designs for the next iteration. (c) direct inverse design, where optimal design will be generated directly from target properties in an iteration-free manner.

etc. Section 2.1 discusses different multi-material topology optimisation (MMTO) approaches. The optimisation workflow in such numerical methods follow a forward and iterative process (Figure 2a). Section 2.2 focuses on ML-based inverse design methods. ML helps to accelerate design evaluation or alters the workflow into a reverse and iteration-free manner (Figure 2b,c).

2.1. Numerical methods: multi-material topology optimisation

TO aims to strategically allocate materials within the design domain according to pre-defined objectives and constraints. A typical example in structural application is to minimise compliance (i.e. maximise stiffness) whilst abiding the volume fraction (VF) constraint. Numerical techniques, such as finite element (FE) analysis, were utilised to model the structural behaviour, where input information includes material properties, loading and boundary conditions. In each iteration, the sensitivity of the objective with respect to design variables will be calculated, guiding the next iteration of design updates until convergence.

In the density-based and evolutionary method, the design commonly adopts a pixel/voxel representation, which allows free reallocation of materials within a discretised domain. Conversely, solutions offered by the level set (LS) are characterised by material boundaries. Alternating active phase (AAP) algorithm tackles the multi-material problem from a different perspective by iteratively calling a binary-phase solver over all the dual-material combinations. To clarify the terminology, when counting the number of material phases in the MMTO algorithm, the convention is to include both the void region and all the solid material candidates. Therefore, 'binary-phase' corresponds to 'single-material'. For an overview of binary-phase TO methods, please refer to the comparative studies conducted by Sigmund and Maute [42]. Table 1 provides a high-level overview of the MMTO methods along-side outlining their strengths and weaknesses.

2.1.1. Density-based method

Solid Isotropic Material with Penalisation (SIMP) approach was introduced by Bendsøe [43], which relates effective material properties to elemental relative densities using the power law relationship, as shown in Equation (1). At conception, this was a two-phase optimisation problem – a single material phase plus a void phase.

$$\text{SIMP: } E_i = x_{i1}^p E^{(1)} \quad (1)$$

Table 1. Overview of MMTO methods.

MMTO method	Description	Advantages and limitations
Density-based	Material distribution is represented as a continuous density field over a discretised domain. Effective properties are defined by material interpolation schemes (SIMP, RAMP)	Compatible with gradient-based solvers Ambiguity in material assignment due to intermediate densities
Evolutionary	The discrete material distribution is iteratively updated based on sensitivity rankings	Discrete design variables result in binary material assignment The heuristic nature limits scalability
Level set	Material boundaries are determined by sign combinations of multiple level set functions, typically evolving based on shape sensitivities	Smooth and clearly defined boundaries, suitable for interface modelling Challenging to handle complex topological changes and high dependency on design initialisation
Phase field	Equivalent to solving a dynamic phase transition system, with energy terms promoting phase separation and interface regularity	Computationally expensive due to additional field equations
Alternating active phase algorithm	Decompose into a series of binary-phase problems, then couples these partial solutions using an outer iteration strategy	Leverages existing binary-phase solvers with minimal adjustment Computational overhead with increasing material phases

SIMP approach was first extended to three-phase optimisation by Sigmund [44] in 1996 when designing composites with extremal thermal expansion coefficients. The key difference between single and multi-material density-based TO lies in the formulation of the material interpolation scheme. This work adopted the recursive multiphase materials interpolation (RMMI) scheme. Element-wise, each design variable corresponds to the presence of one material type, shown in Equation (2).

$$\text{RMMI – SIMP: } E_i = x_{i2}^p (x_{i1}^p E^{(2)} + (1 - x_{i1}^p) E^{(1)}) \quad (2)$$

Uniform multiphase material interpolation (UMMI) scheme is also prevalent in literature, owing to its benefits of linearity and variable separability. In contrast to the recursive formulation, the effective property is a weighted sum of all the material candidates, shown in Equation (3). Different expressions exist for the weighting functions in UMMI.

$$\begin{aligned} \text{UMMI – SIMP: } E_i &= \sum_{j=1}^m w_{ij} E^{(j)} \\ &= x_{i1}^p E^{(1)} + x_{i2}^p E^{(2)} \text{ when } w_{ij} = x_{ij}^p \end{aligned} \quad (3)$$

A comparison between RMMI and UMMI could be found in [45], within the context of a mass-constrained structural optimisation problem. Since the power law relationship is present in both RMMI and UMMI, they are generally referred as the ‘modified power law approach’ in literature and serve as the fundamental theory in the multi-material SIMP approach.

Rational Approximation for Material Properties (RAMP) is another density-based TO method wherein the effective property is related to the design variable as shown in Equation (4) [46].

$$\text{RAMP: } E_i = \frac{x_i}{1 + q(1 - x_i)} E^{(1)} \quad (4)$$

Similar to the exponent term p in SIMP, the parameter q penalises intermediate density in RAMP. Some intriguing characteristics of the RAMP model are that it yields non-zero sensitivity at all values of the design variables, especially at $x = 0$, and the objective function is convex for certain selections of q . RAMP method was first generalised to an arbitrary number of material phases by Hvejsel et al. [47] and it is challenging to formulate the scheme recursively; thus, UMMI is the dominant approach.

$$\text{UMMI – RAMP: } E_i = \sum_{j=1}^m w_{ij} E^{(j)} \text{ where } w_{ij} = \frac{x_{ij}}{1 + q(1 - x_{ij})} \quad (5)$$

The outputs of density-based MMTO are continuous relative densities between 0 and 1 for each material candidate, in which the manufacturing implication of intermediate densities remains unclear. Research effort has been made to develop novel material interpolation

schemes that polarise intermediate-density elements. For example, a modified volume-preserving Heaviside function [48] was utilised by Yan et al. [49] to promote clear boundaries of material choices in a multi-scale thermoelastic lattice structure design case. Cui et al. [50] adopted logistic functions such that design variables were computed proportional to elemental compliance or stress, however, sensitivity calculations were eliminated during the optimisation process to reduce computational cost. Yi et al. [51] formulated the interpolation function as the design variable multiplied by the ratio of the p -norm to the l -norm, promoting definitive material type at each element.

MMTO inherently poses a computational challenge – the number of design variables scales up with the number of material phases. To overcome this, a peak function material interpolation model was developed by Yin et al. [52], encompassing a linear combination of normal distribution functions. However, the presence of zero gradient introduces numerical challenge in transitioning between material phases. The ordered SIMP model proposed by Zuo et al. [53] also tried to model the multi-material topology with single variable to save computational cost. As illustrated in Figure 3(b), scaling and translation coefficients were populated to construct a piecewise interpolation function with respect to the normalised density variables, where the number of subdomains matches the number of solid materials. Similarly, Zhao et al. [54] utilised an ordered RAMP model to tackle non-probabilistic reliability-based MMTO with evidence theory. These ordered single-variable interpolation methods have been applied to solve mass or stress-constrained problems

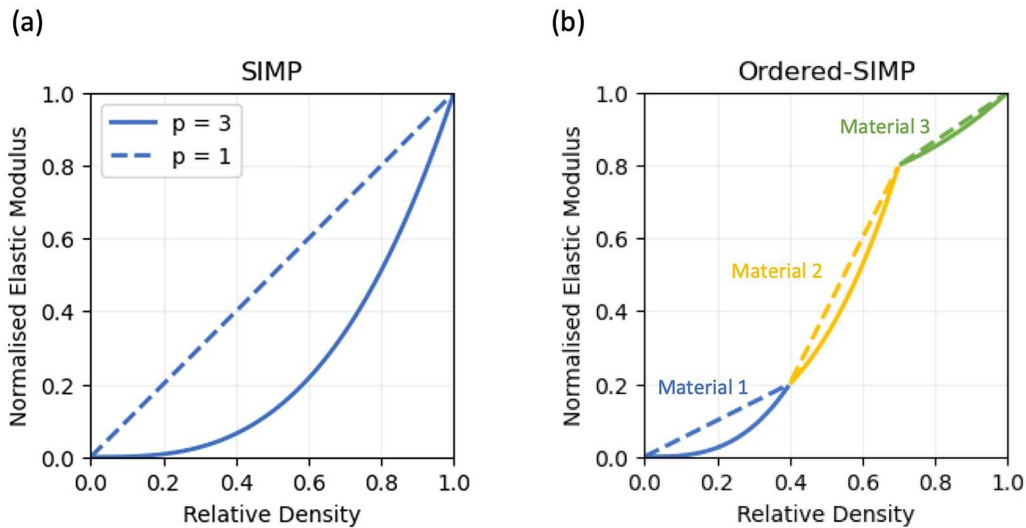


Figure 3. Comparison of the material interpolation scheme and the effect of penalisation. (a) Conventional SIMP with a solid phase and a void phase. (b) Ordered-SIMP with three solid materials, adapted from [21].

[55–57], as well as robust optimisation under load uncertainty [58,59].

The inclusion of multiple materials increases complexity in the optimisation problem. Consequently, effecting numerical stability and robustness. The ranges of the effective property are restricted by Hashin-Shtrikman (HS) bounds [60], which were reflected by the choice of the exponent in the power law expression in the SIMP method. Sigmund [61] proposed to use a weighted average of the HS upper and lower bounds, such that the discontinuity in properties between two material phases could be eliminated with a smooth HS interpolation. The optimisation of a non-convex function is susceptible to local optimum. By introducing reciprocal variables into SIMP formulation, the original model could be reformulated into a sequential quadratic programming problem, mitigating the risk of suboptimal solutions [62].

Greater design freedom afforded by MMTO enables superior solutions to be explored within a multi-objective context (e.g. mechanical and thermal). The objective function is commonly expressed as a linear weighted function of several conflicting objectives. Kruijff et al.'s work [63] examined the topological transition by changing the weights while Vantghem et al. [64] conducted parametric studies to analyse the effect of property disparity between material candidates. Chen et al. [65] considered temperature-dependent thermoelastic properties, applicable to thermally sensitive multi-material applications. Another research perspective is to design metamaterials with tunable thermomechanical properties [66–68], such as negative Poisson's ratio (ν), and zero/negative/anisotropic coefficient of thermal expansion (CTE). With respect to thermal buckling, Wang et al. [69] optimised the buckling capacity with decoupled mechanical and thermal loading while Wu et al. [70] formulated the problem as minimising the total volume of all the materials subject to thermoelastic compliance and buckling constraint. In addition to the steady-state analysis, transient heat conduction was addressed by Li et al. [71] under functional gradient constraint, and by Nguyen [72] under specific frequency constraints.

2.1.2. Evolutionary method

In contrast to density-based TO, the type of design variables in the evolutionary method is discrete (i.e. 0 or 1). Bi-directional Evolutionary Structural Optimisation (BESO), proposed by Yang et al. [73], is the most well-known approach and successor to the Evolutionary Structural Optimisation (ESO) [74]. The term 'bi-directional' implies that elements could not only be removed but also added when certain conditions were satisfied.

The work conducted by Huang and Xie [75] formed the foundation of MM-BESO. Essential steps in MM-SIMP such as material interpolation, sensitivity calculation, and filtering techniques, are all present in MM-BESO, while the key difference is that intermediate densities were not allowed. Ghabraie [76] suggested to replace the penalty factor with a filtering scheme, in which element sensitivities were multiplied by their elastic moduli, aiming to eliminate numerical anomalies encountered in multi-material problems. Li et al. [77] later revised the material allocation rule from sensitivity ranking to computing the sum of principle stresses, reflecting the potential difference in tensile and compressive properties (Figure 4a). This characteristic is especially important in designing concrete-based civil applications such as bridges [78,79] (Figure 4b) and long cantilevered buildings [80] – both multi-material. Structural safety was further improved by adding reinforcement to regions with overloaded compressive stress [81] (Figure 4c). Attempts have also been made to distinguish tensioned and compressed elements, subsequently allocating high – and low-rigidity materials at each region [82]. Beyond generative design, a cable-supported bridge prototype has been constructed and validated via 3D concrete printing [83], illustrating the feasibility of MMAM in the construction industry.

To summarise a few design cases, Radman et al. [84] employed BESO to design multi-phase period microstructures with maximum stiffness or thermal conductivity. Xia et al. [85] optimised quasi-brittle composites by maximising fracture resistance. Zheng et al. [86] considered interval loading uncertainty in designing robust multi-material structures. Graded interface was also investigated by Han et al. [87], in which an extended-BESO method helped to avoid the stress singularity. Liu et al. [88] adopted RMMI for discrete variables and demonstrated its superiority against continuous variables in minimising compliance under total mass constraint. Conceptually, the MM-BESO framework can solve diverse optimisation problems, but its utilisation is relatively limited compared to MM-SIMP. This could be attributed to the convergence challenge and the high computational cost in sensitivity sorting associated with discrete design variables.

2.1.3. Level set method

LS method belongs to the boundary-based TO framework, where the structural configuration is represented by the iso-surface of a LS function in a higher dimension space [89]. During the optimisation process, the external shape of the LS function will be updated based on the distribution of shape derivatives [90]. Alternatively, the update could rely on topological derivatives whereas



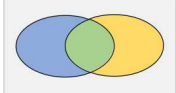
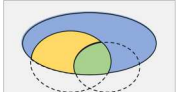
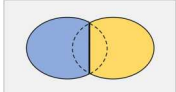
the LS function mainly serves as a topology representation [91].

Among existing LS schemes, the colour level set (CLS) and multi-material level set (MMLS) methods are the most widely applied in designing engineering applications (Figure 5). The CLS method has been utilised not only in structural design, such as compliant mechanisms [94,95], but also in applications involving other physics, including elastic and thermoelastic structures [96,97], heat conduction devices [98], and flexoelectric composites [99]. The MMLS method is

2.1.4. Phase field method

In the phase field method, the optimisation process of a multi-material solid structure can be treated as a dynamic phase transition system, in which the solidification stage implies a convergence to the optimised topology. Mathematically, the TO problem was transformed into solving a set of fourth-order nonlinear parabolic partial differential equations (PDE). Zhou et al. [123] applied the Cahn–Hilliard theory to construct a modified thermodynamic model consisting of three energy components. The bulk energy and interface energy reflect the incorporation of multiple materials whilst the elastic strain energy is the major driving force of

Table 2. Overview of multi-material level set schemes.

MMLS scheme	Material assignment rule	Figure / Equation	Advantages and limitations	Application to design case
Partitioning	Each LS function represents a distinct solid material [92]	 $n = m + 1$	Requires additional constraints to prevent phase overlap; otherwise, interpolation schemes are needed for overlapped regions.	
Color	Defining the intersection of any two zero LS contours as a new material structural domain [93]	 $n = 2^m$	Substantially reduce the computational cost when the number of material increases ($n > 3$)	[94–99]
Multi-material	Introducing a new material region as the intersection of the new zero LS contour and all the existing ones [100]	 $n = m + 1$	Naturally avoids overlapping or redundant regions. Explicit mathematical expression facilitates sensitivity analysis.	[101–110]
Piecewise constant	Each material phase is represented by a unique constant in a piecewise constant LS function [111]		Boundary description by discontinuities of the piecewise constant LS function rather than solving the Hamilton-Jacobi equation. Improved storage capability and enabled complex geometry generation [112]	[113]
Reconcile	Reconcile the overlapped LS fields with the Merriman-Bence-Osher (MBO) operator [114]	 $n = m + 1$	Preserves the one-to-one relationship between LS functions and materials, as well as the signed distance concept	[115,116]
Vector-valued	Represent n phases by a vector-valued LS function mapping into $\mathbb{R}^{n-1}$ [117]		Design update only relies on topological derivatives. Eliminates the need for a perforated initial design with the incorporation of a hole nucleation mechanism	
Extended	In a matrix-valued function, each element is a scalar LS function representing the boundary between two phases [118]	 $m = n^2$	High degree of freedom during optimisation, less dependency over initial configuration, and simple topological derivative calculation with the reaction-diffusion equation, with the trade-off being computational time	[119–122]

Note: The elliptical shape represents the zero iso-surface of a LS function. The number of LS function is denoted by m , and the number of material phases is denoted by n . Each material phase is presented by a unique color, and the void phase is shown in grey.

compliance minimisation. With increasing iterations, the phase-field method promotes the coalescence of initially dispersed regions of the same material into larger, contiguous domains (see examples in [123]). This behaviour reflects the interface-regularising nature of the phase-field method and is not typically observed in density-based approaches.

Multi-material phase field method have been extended to tackle problems with non-linear deformation [124], regulate elastic bodies in unilateral contact [125], and conduct multiscale concurrent optimisation of porous structures [126]. Engineering applications designed under this approach include vibrating structures [127], shape-morphing electroactive polymers [128] and other general 4D printing devices [129].

2.1.5. Alternating active phase algorithm

The AAP algorithm was proposed by Tavakoli et al. [130] as a new perspective to tackle MMTTO problems. Rather than solving for multi-material directly, AAP splits a multi-phase problem into a series of binary-phase sub-problems, then couples these partial solutions using an outer iteration strategy (Figure 6a). Specifically, only two material phases out of n will be activated during each subproblem, while the topologies of the rest ($n - 2$) phases remain fixed (Figure 6b). The distribution of the two activated phases could be determined using a well-developed single-material TO algorithm. Most literatures employed SIMP-based internal solver while a few used LS method [131,132], but technically, the internal solver is not restricted to any specific TO methodology. Then,

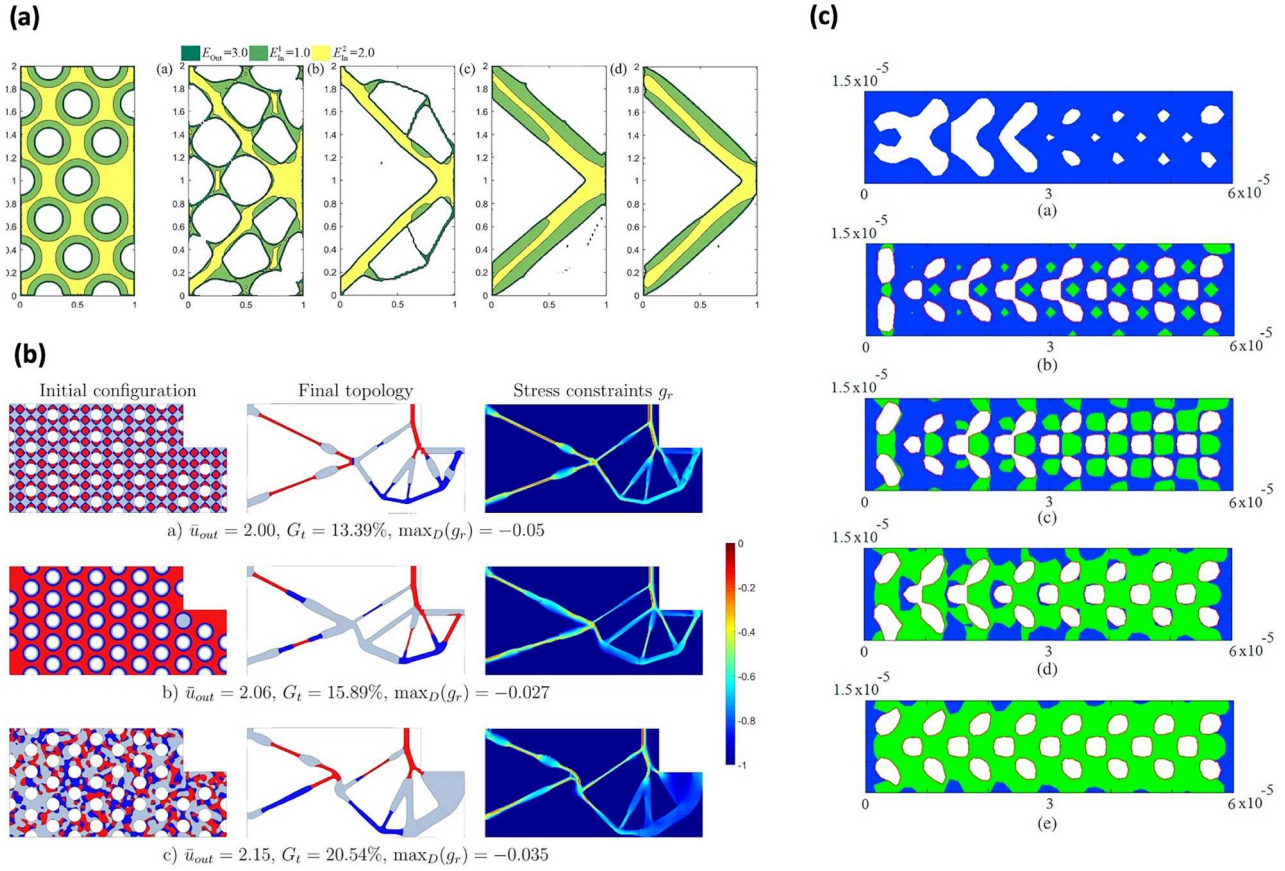


Figure 5. Numerical examples of multi-material level set method. (a) Iteration history of a multi-material coated two-bar cantilever. Reprinted from [110] with permission from Elsevier. (b) Gripper mechanism considering stress constraints. Reprinted from [105] with permission from Elsevier. (c) Flexoelectric beam consists of active (blue) and passive (green) materials. Optimised under different volume fraction constraint using the colour level set scheme. Reprint from [99] with permission from Elsevier.

the outer iteration was structured based on the block coordinate descend method. Following the combinatory mathematics rule, the number of sub-problems in each iteration step equals $nC_2 = n(n-1)/2$, and the optimisation will stop until global convergence.

Overall, the generality of AAP is reflected by minimal adjustments required to existing binary TO solvers, and the ability to preserve these solvers' capability in addressing specific objectives or constraints. However, the computational cost rises significantly with increasing material candidates. Huamani et al. [133] improved this aspect by adopting a non-monotonic spectral projected gradient method, such that the number of sub-problems was reduced to n and the convergence became independent of the filter radius. Yan et al. [134] proposed an enhanced AAP algorithm where penalty threshold and steepness factor were added to the material interpolation scheme, such that the degree of penalisation becomes adjustable between high – and low-density elements to facilitate convergence.

The AAP framework, with its update scheme specifically developed for multi-material, was applied to solve

optimisation problems with diverse engineering objectives. In designing shape-morphing structures with tunable ν and CTE, Han et al. [135,136] addressed the convergence oscillation problem in AAP by dynamically switching the objective function based on the current active material phases. A material distribution-based cluster method was proposed to address local stress concentration rather than a global constraint [137], reflecting differences in material strength. Studies also proved that multi-objective optimisation considering stress [138] or material cost [139], robust optimisation considering load uncertainty [140], and length scale control (LSC) for orthotropic multi-material structures [141] could also be solved under the AAP framework.

2.1.6. Other numerical methods

In the moving morphable component (MMC) approach, the design is defined by a set of morphable building blocks and then optimising their layout and geometric parameters based on sensitivity analysis. By assigning different material properties to those structural components, MMC could be readily extended to multi-

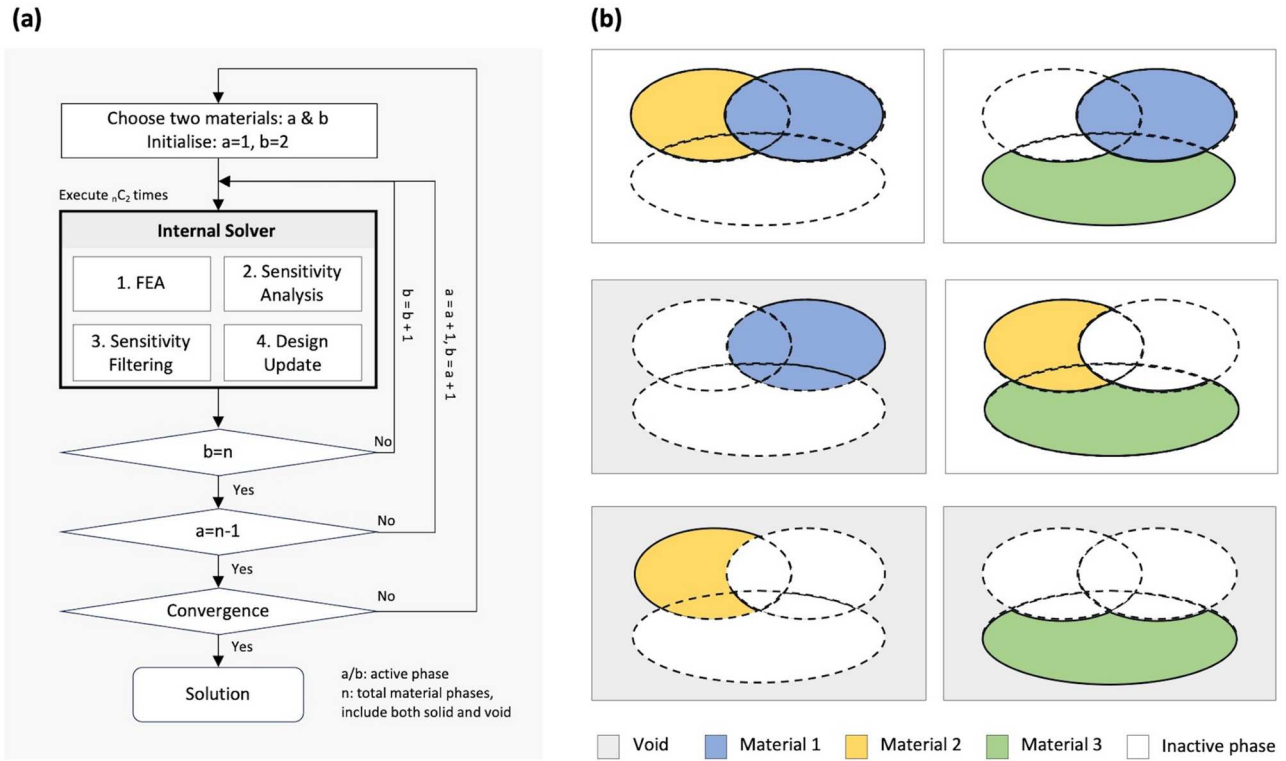


Figure 6. Alternating active phase algorithm. (a) Flowchart of the AAP algorithm involving the outer iteration and the internal binary-phase solver. (b) Alternation of active and inactive phases for a four-phase topology optimisation problem based on the multi-material level set scheme, adapted from [132].

material with significant savings in design variables compared to MM-SIMP [142]. The moving morphable voids (MMV) method has a similar problem formulation but with voids as explicit geometric descriptors instead [143].

Besides gradient-based optimisation, FE analysis could also be integrated into evolutionary algorithms, playing the role of fitness evaluation for design candidates. This heuristic approach has been adopted in designing multi-material structures with desired deformation behaviour [144,145]. Other numerical techniques, such as linear or quadratic programming, are conceptually feasible but rarely attempted unless the combinatory design domain is very small, and simultaneously the optimisation objective formulation does not involve higher-order operations.

2.1.7. Benchmarking representative MMTO methods

Three representative MMTO methods are selected for comparison: (1) MMLS scheme [100], (2) MM-SIMP with a mapping-based interpolation function [146], (3) AAP algorithm with a SIMP-based internal solver [130]. The design in MMLS scheme is boundary-controlled while the latter two methods adopt voxel-based representations. Figure 7(a) outlines the detailed setup of the two-material cantilever beam example. The optimised

solutions adopting each method are demonstrated in Figure 7(b–d), along with the iteration history on optimisation objective and VF constraints, as well as the visualisation of intermediate solutions.

The MMLS scheme (Figure 7b) results in the lowest compliance as desired, while the other two voxel-based methods have comparable performance. Iteration history of VF demonstrates a convergence trend to the target values after 20 iterations despite initial fluctuation. The authors who proposed the MMLS scheme [100] claimed that the design must be initialised with a reasonable number of holes to ensure a desired resolution. Indeed, high dependency on design initialisation is a general trend in LS methods despite the specific multi-phase schemes used. The manufacturing implication of the MMLS method is straightforward as material boundary is clearly defined. However, significant amount of multi-material interface is present since the weaker material did not form independent loading paths by itself. Moreover, explicit LSC strategies must be incorporated to regulate the feature size to a manufacturable standard.

For the AAP algorithm (Figure 7d), the compliance and VFs all stabilise after 20 iterations from a uniform design initialisation. However, intermediate densities in the optimised solution led to blurry regions and ambiguity in

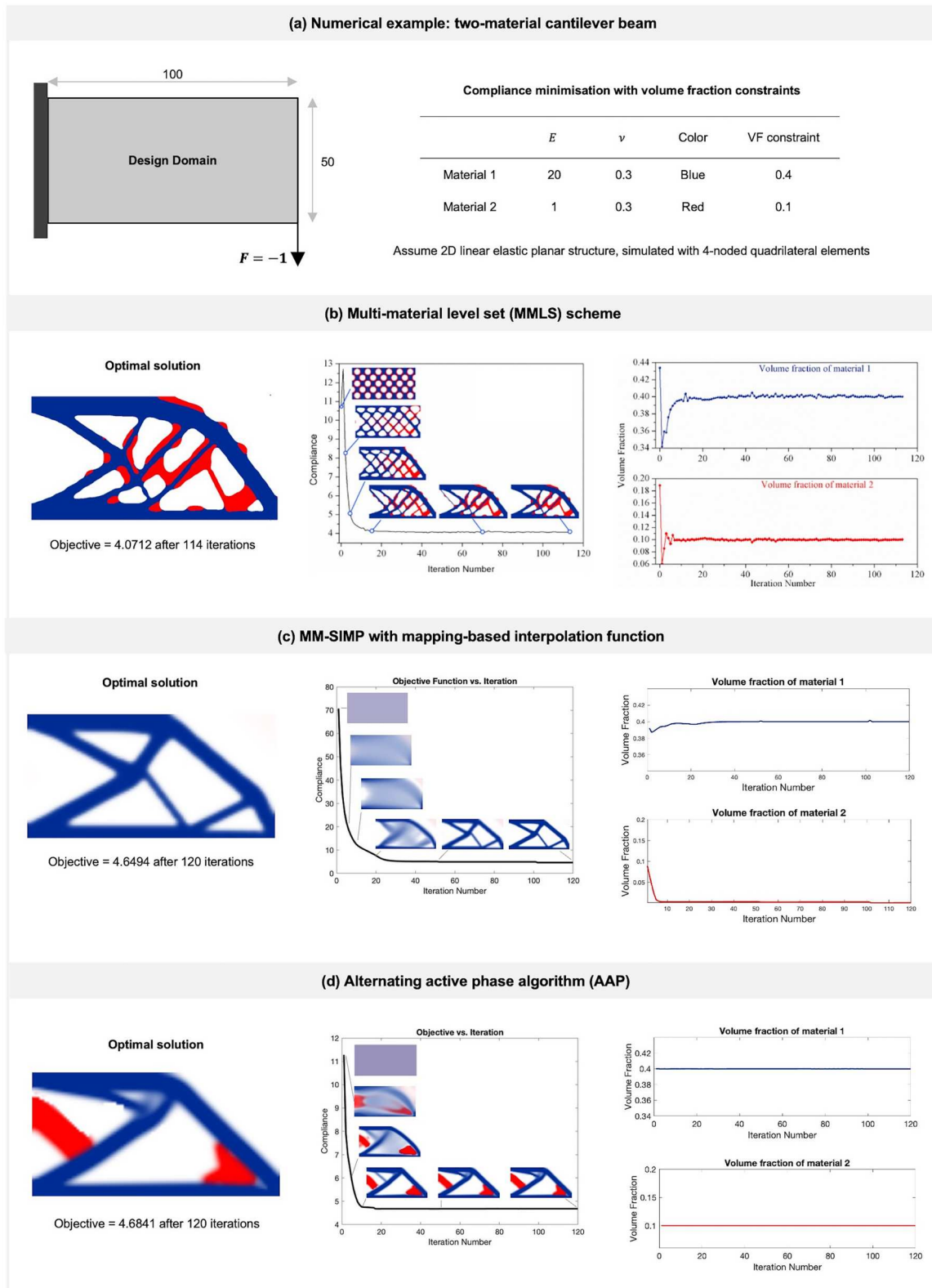


Figure 7. Benchmark three representative MMTTO methods with a two-material cantilever beam design case. Aspects of comparison covers the optimised solution, convergence of the objective function and VF constraints, and visualisation of intermediate solutions. (a) Details about the two-material cantilever beam optimisation problem. (b) Results adopting the multi-material level set (MMLS) scheme. Reproduced from [100] with permission from Elsevier. (c) Results utilising the MM-SIMP method with a mapping-based interpolation function. Data generated from the open-source code [146]. (d) Results applying the alternating active phase (AAP) algorithm. Data generated from the open-source code [130].

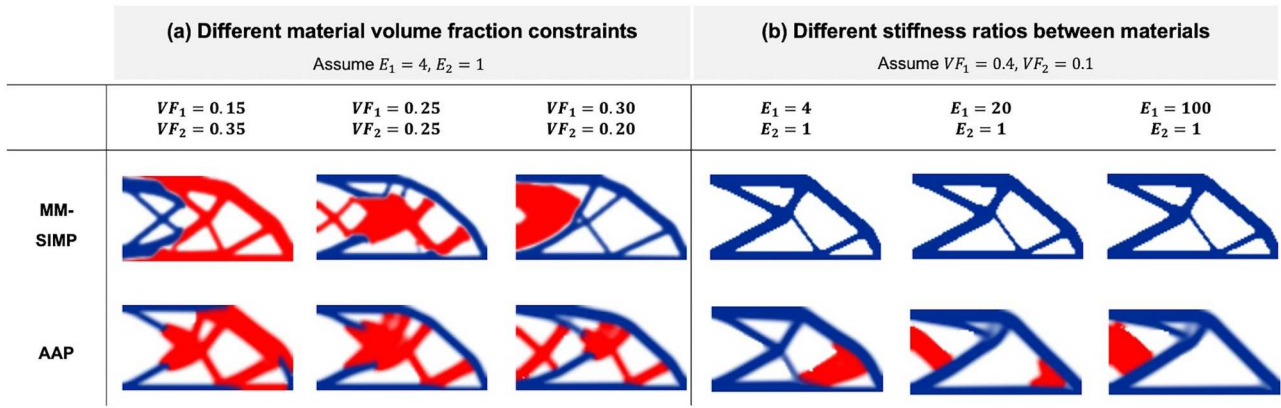


Figure 8. Benchmark two representative voxel-based MMTTO methods: (a) under different material volume fraction constraint. (b) with different stiffness ratios between materials. Results for MM-SIMP and AAP are generated from code [146] and [130], respectively.

allocating materials. In general, voxel-based design representation is less dependent on design initialisation but more sensible to parameters such as filter radius. Regarding the MM-SIMP method (Figure 7c), it is observed that the second material was gradually eliminated within the first five iterations, resulting in a single-material solution that significantly violates VF constraint. Additional examples were provided with different VF constraints and stiffness ratios (Figure 8) to assess whether this trend is consistent. It turns out that a material phase with both low VF and significantly lower stiffness tends to be eliminated during the optimisation process. Note it is likely contributed by the optimiser – Method of Moving Asymptotes (MMA) – rather than generalisable to MM-SIMP formulations.

Computational time required for optimisation is rarely reported across literature. It is influenced by factors such as design size, mesh resolution, and number of materials. Most numerical studies adopt 2D domains with up to three materials, leaving scalability with design dimension and material count unclear. Nevertheless, graphics processing unit (GPU) acceleration offers a promising solution, as demonstrated in various single-material TO frameworks already. Some focused on building efficient GPU-based FEA solvers utilising matrix-free conjugate gradient methods and multi-grid approaches [147,148]. Others have explored modularising the TO pipeline to evaluate different CPU-GPU configurations [149,150]. While above-mentioned strategies show promise in improving computational efficiency, none have yet explored their application in the multi-material context, presenting an opportunity for future research.

2.1.8. Selection of MMTTO methods aligned with MMAM design aspects

In selecting computational design tools for multi-material structures, it is essential to align the method

with specific design aspects outlined in Figure 1. To provide a general comparison, MMTTO methods are grouped into two broad categories based on design representation: voxel-based (e.g. SIMP, RAMP, BESO) and boundary-controlled (e.g. LS). The baseline that assumes the least computational design complexity, is characterised by discrete material composition, 2D design domain, planar layering, and mono-scale structures. For each aspect, remarks are provided to assess the feasibility of extending the respective MMTTO methods to accommodate advanced multi-material design complexity.

Most existing computational design methods assume discrete material composition where perfect bonding exists at distinct material interfaces. The number of material choices rarely exceeds three, representing the state-of-the-art in manufacturing and constrained by the computational burden. Although imperfect interfaces are commonly observed in experiments, only a few works in MM-SIMP and MM-LS have attempted to model them, to be elaborated in Section 5.1. Notably, smooth property gradation – rather than abrupt transitions – has been implemented locally at material interfaces in both methods. These graded zones are typically confined to narrow interfacial regions, with widths much smaller than the overall structural scale.

Continuous composition relaxes the above-mentioned finite material choice constraint by considering spatially varying material mixture ratios, enabling infinite number of material choices and omitting interfacial concerns. Its computational implementation is, however, commonly realised by approximating with discrete composition at a smaller scale [151]. Therefore, voxel design representation is more suited to reflect macroscale continuous composition while boundary-controlled methods inherently divide the design into discrete material domains. As future work, compatibility

and property characterisation for the material mixture requires further experimental investigation to ensure accurate modelling.

The most free-form output of a computational design algorithm possesses intra-layer multi-material capability, that is, several materials including voids are allowed within each layer. Additional constraints need to be implemented to realise inter-layer restriction imposed by the fabrication technique. Since layers are easily distinguishable in a voxel design representation, applying the constraint might be numerically demanding but practical. Conversely, it is infeasible for boundary-controlled design to follow alternating material layout. Composite laminates can be treated as a special type of inter-layer multi-material structure, where property variation is introduced by changing the fibre orientation. Its optimisation focuses on the stacking sequence and layer thickness while preserving topology along the building direction. Discrete Material Optimisation (DMO) is a technique dedicated to this kind of design scenario [152,153].

A cartesian coordinate system is the default option in both computational design and manufacturing processes, resulting in a planar printing layer unless otherwise specified. Multi-axis robotic arms or build platforms with rotational degrees of freedom provide flexibility in depositing materials on non-planar surfaces. Non-cartesian designs can be adapted for planar fabrication by slicing into planar layers, but this sacrifices direction-dependent properties.

When the dimension is restricted to 2D in computational design, the printed part will maintain a consistent geometry and material in the building direction (i.e. 2.5D planar extrusion). Expanding to 3D enlarges the design space for improved optimisation but requires addressing printability and support structures. Voxel-represented design methods are more readily extendable to 3D, where the mesh resolution should be taken into consideration to avoid computational burden. The combination of active and inactive material also enables 4D printing, where the fourth dimension refers to time-dependent shape change. The shape morphing capability could be triggered by environmental stimuli such as change in temperature [154,155] or pH level [156].

MMTO typically outputs mono-scale structures, but voxel-based representation facilitates multi-scale extensions more readily than boundary-controlled methods. Although most multi-scale designs involve two levels (i.e. micro – and macro-) to be optimised concurrently or sequentially, hierarchical structures with additional scales are also feasible [31]. The computational cost becomes a concern when designing the micro – and macro-structure with the same length scale in MMLS method. Guyan reduction method was investigated by

Chung et al. [157] to address the challenge. Physical length scale is crucial for manufacturability, where existing control strategies are mainly explored within voxel-based design methods (Section 5.3.1).

2.2. Machine-Learning-Based methods: inverse design

Depending on the design workflow shown in Figure 2, computational methods that utilise ML models have been divided into two categories: (i) direct and (ii) indirect. Direct inverse design is an iteration-free approach, as the mapping between properties and design parameters was established typically using generative models such as variational autoencoder (VAE) or generative adversarial networks (GAN). In indirect inverse design, predictive models, such as multi-layered perceptron (MLP) or convolutional neural networks (CNN), were trained to forecast properties from a given design representation. Since the property predictor enabled faster feedback during design space exploration, a genetic algorithm could be utilised to find the best-matching candidate.

As dataset preparation is an essential step in training models, ML-based methods are commonly referred as the data-driven approach. Note that the optimiser in the gradient-based TO framework (i.e. optimality criteria, MMA) may be replaced by neural networks (NN). However, since only a few researchers investigated this perspective under the multi-material context [158–160], the following sections will mainly focus on ML's capability in surrogate modelling and generative design.

2.2.1. Direct inverse design

Direct inverse design is a strategy to generate solutions from target properties or performance in an iteration-free manner. This is achieved by training an ML model that directly captures the relationship from the supplied dataset. Teawdeswan et al. [161] aimed to design gyroid structures made of PLA and TPU with tunable compression behaviours (Figure 9a). Experiments were first conducted by varying the percentage of PLA and the relative density of a unit cell, obtaining properties of interest (E , energy absorption and the peak stress). Interpolation functions were constructed and served as the ground truth in training a feedforward NN that outputs design parameters given compression behaviour requirements.

Zeng et al. [162] employed a pixel metamaterial design method that mapped $E - G - \nu$ mechanical property space into R-G-B colour space for each unit cell, consequently accelerating the macro-structure design of an implant by rapid micro-structure

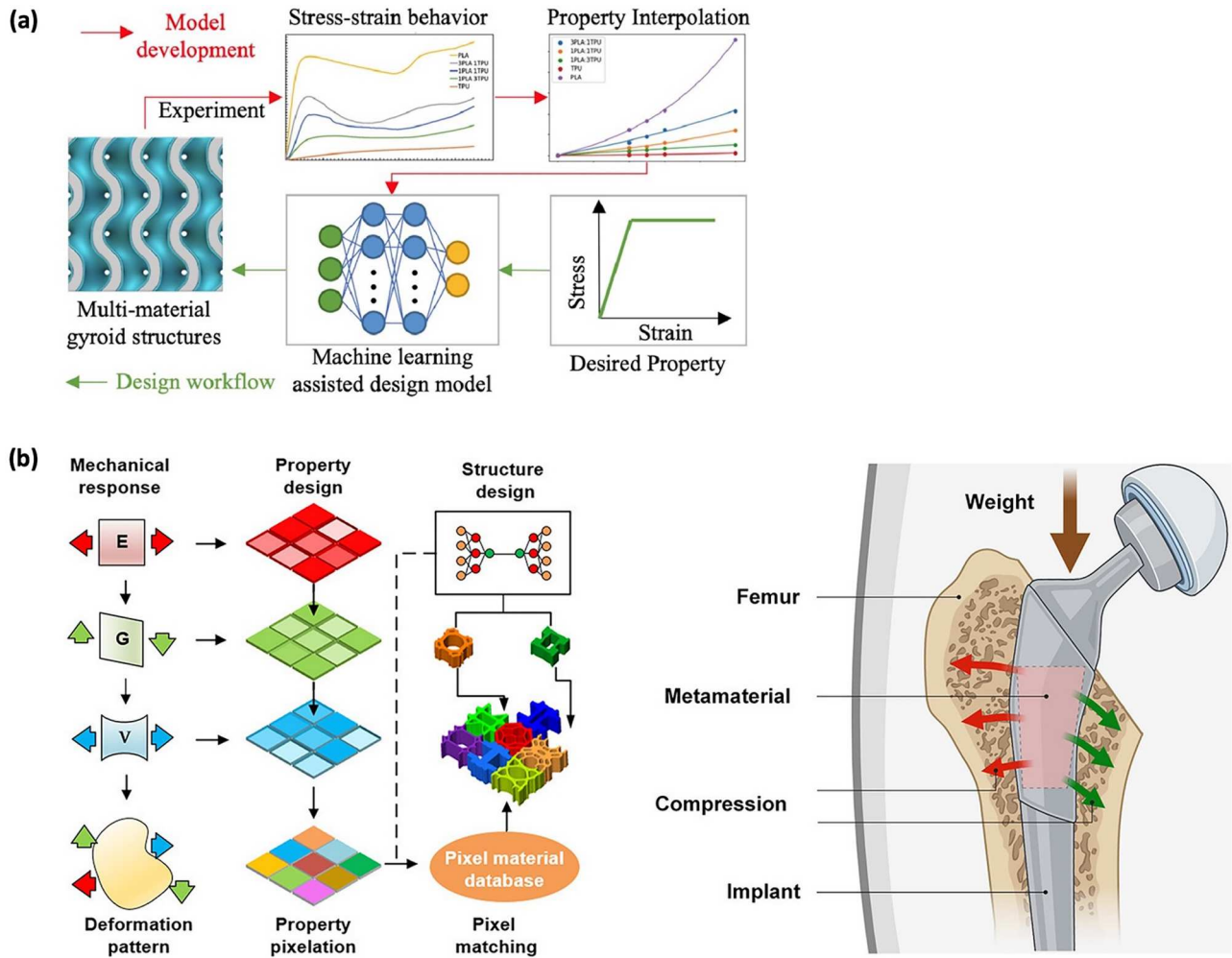


Figure 9. Multi-material design adopting the direct inverse design strategy. (a) Optimise multi-material gyroid structures given desired stress-strain behaviour, reprinted from [161] with permission from Elsevier. (b) Multiscale design of functionally graded meta-materials and its application in human hip joint design, reprinted from [162] with permission from Elsevier.

generation (Figure 9b). To achieve this, both the property predictor and the structure generator adopted an encoder-decoder configuration, while GANs were utilised to supplement the database. Li et al. [163] extracted the generator of a well-trained ResUnet-GAN model for the multi-material structural design task, while MM-SIMP was adopted to prepare the training dataset.

Video diffusion models were leveraged by Park et al. [164] to generate mechanical solution fields from non-linear stress-strain responses. Two consecutive UNets then post-process the solution fields: the first segments solid and void regions, and the second classifies material choices. Dimassi et al. [165] developed a computer-aided design plugin that suggests the distribution of active and passive materials given the desired shape change. A semantic similarity vector space model was trained, showing the potential of natural language processing techniques in multi-material design.

2.2.2. Indirect inverse design

Indirect inverse design method evaluates performance metrics with predictive ML models. The aim is to replace numerical analysis, which is typically the most time-consuming step within the optimisation workflow. Table 3 summarises various ML models used for prediction tasks, emphasising that model selection should align with the format of multi-material design inputs and target properties. Although the predictor by itself does not provide design solutions directly, the prediction accuracy does influence ultimate design quality. Moreover, the diversity of the predictor determines which property criteria the inverse design generator may impose. Therefore, the strategies applied are still insightful and transferable to the complete inverse design framework.

A genetic algorithm could be adopted to search the optimal multi-material design parameters, where fitness evaluation or constraint checking could be

Table 3. Summary of property prediction using ML models in multi-material design.

Design parameters	Predicted properties	ML model	Reference
Specimen height, coating and base thickness, shore hardness of cost/base layers, infill type	Effective shore hardness and compressive modulus of PolyJet printed parts that mimic human tissues	MLP	[166] *
Microstructure defined by curvature functions and graded material composition. The axial strain.	Tensile stress, Poisson's ratio, the lateral profile of the deformed shape	MLP	[167] *
Multi-material distribution in pixel format	Energy conversion factor, electric field, and deflection due to flexoelectricity	MLP	[168] *
Material assignment of each strut in a tessellated lattice structure and the unit cell angle	Elastic modulus and Poisson's ratio in two orthogonal directions	MLP	[177]
Fibre size variables and rotation angle of functionary graded composite	Anisotropic homogenised elasticity tensor with nonlinear behaviour	MLP	[178]
Graded material composition of PLA and TPU	Fatigue cycle of polymetric functionally graded materials manufactured by material extrusion	RF, SVM, MLP	[169]
Multi-material distribution in pixel format	Displacement field under total mass constraint	CNN	[170] *
Multi-material distribution within a ¼ unit cell in pixel format	Stiffness, Poisson's ratio	CNN	[171] *
Cross-sectional image of an interior permanent magnetic motor	Magnet flux and dq-axes inductance to compute the average torque	CNN	[172]
Five geometric parameters defining the distribution of TPU and Nylon at the beam's cross-section	Beam deflection under three-point bending	Bayesian	[173]

Note: * indicates the study has been extended into an indirect inverse design framework with genetic algorithm, while the rest are standalone training of the property predictor.

conducted via the pre-trained ML models. Goh et al. [166] aimed to mimic human tissue properties by layering composites with coat, base, and infill materials. Shore hardness and compressive modulus were predicted via a shallow neural network, where material and geometric information serve as the five input parameters. Also enabled by an MLP model, Dong et al. [167] inverse designed multi-material lattice structures with customisable stress state, ν , and lateral deformation profiles. The microstructure was characterised by curvature functions and the percentage of soft/hard materials (Figure 10a). Hamdia et al. [168] designed nanostructures made of elastic and flexoelectric materials, where an MLP model was used to forecast energy conversion factor, electric field, and deflection due to flexoelectricity.

Jiang et al. [171] maximised the stiffness of composite structures while maintaining the desired ν . CNNs were chosen for the predictive tasks, since the input format is 16×16 matrices with binary elements, representing the presence of either the stiffer or the soft material at the specified pixel location of a quarter unit cell (Figure 10b). Yang et al. tackled the MMT problem with total mass constraint, where the highlight is that the CNN model was trained based on physics-informed loss function rather than labelled simulation data [170].

2.2.3. Remarks on ML-based methods

ML-based methods offer computational advantages over numerical approaches by replacing costly simulations with predictive models or revising iterative workflows through generative models. However, dataset preparation demands significant computational resources, as obtaining ground-truth properties often requires running thousands of simulations. These

simulations typically involve assumptions such as isotropic material properties, linear elastic conditions, and perfect bonding between materials. Future research is required to assess ML-based methods' capability in moving beyond these assumptions, while keeping the computational time within a reasonable period. Training time depends on dataset size and model architecture, which can be accelerated using GPUs. Once trained, ML models enable rapid design iterations and can easily adapt to different targets, but solution quality remains tied to the dataset's accuracy and diversity.

In contrast to data-heavy approaches, Bayesian optimisation eliminates the need for large datasets by leveraging Gaussian process regression to model the objective function and using an acquisition function to efficiently search for optimal solutions [174]. This makes it particularly suitable for scenarios where objective evaluations are computationally expensive. Existing application of Bayesian optimisation in multi-material design include tailoring composite solids for target elastic moduli [175], predicting beam deflection [173], enhancing crashworthiness of multi-material plates [176], and optimising fingertips for aerial grippers [177].

Physics-Informed Neural Networks (PINNs) not only eliminate the need for labelled training data but also conventional FE analysis. By minimising the residuals of PDEs and boundary conditions, the governing physics are directly embedded into the loss function. With growing research attention, PINNs have been applied to solve static equilibrium [178,179] and diffusion problems [180,181] in multi-material settings. However, a key challenge in multi-material PINNs is accurately capturing discontinuities at multi-material interfaces. To address this, strategies such as domain decomposition [179,181] and enforcing continuity

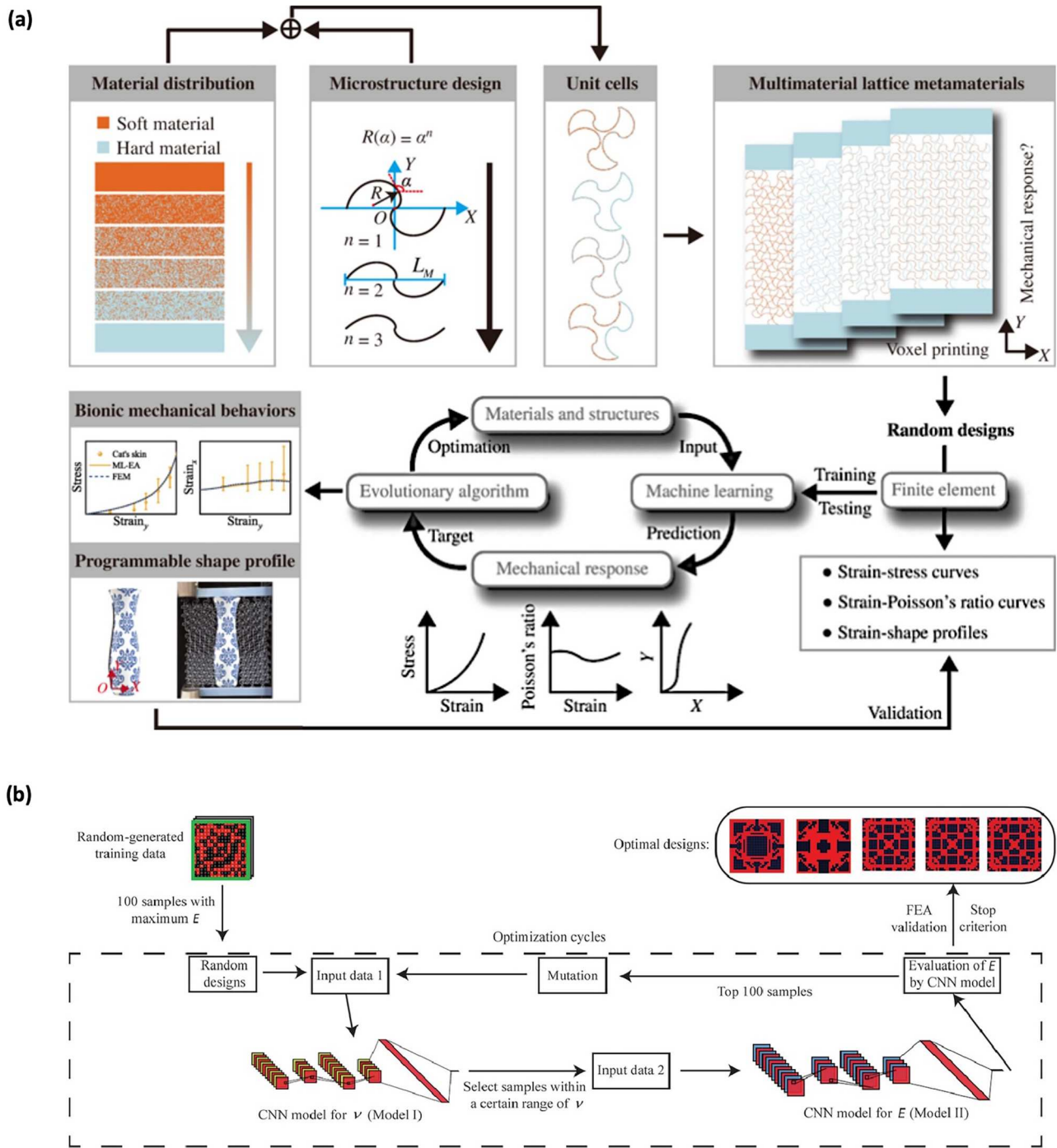


Figure 10. Multi-material design adopting the indirect inverse design strategy. (a) Optimise multi-material lattice metamaterials characterised by hard/soft material distribution and curved microstructure design. Reprinted from [167] with permission from Purpose-led publishing. (b) Training CNN models to predict Young's modulus and Poisson's ratio from pixelated multi-material input. Reprinted from [171] with permission from Elsevier.

through hard constraints [180] have been explored. Moreover, a PINN-based MMTO framework was proposed by Jeong et al. [182], in which structural deformation state and objective sensitivity was predicted via two distinct PINNs. To achieve multi-material design, a classification model was utilised to identify material types across elements.

The choices of ML models must be closely tied to multi-material design representations. MLPs suit parameterised inputs such as graded material composition or categorical labels. CNNs are ideal for voxel-based designs, which offer high design freedom but pose challenges in guaranteeing structural validity. Graph neural networks (GNNs) are well-suited for truss-

based metamaterial, where material properties could be efficiently encoded in edge features. Inverse design remains challenging due to the one-to-many nature of the property-to-design mapping, requiring future research. Techniques to reduce the dimensionality of the design space include applying principal component analysis (PCA) for feature reduction [183] and characterising designs with latent vectors [175].

LSC is less of a concern in inverse design methodologies since the ML model’s predictive or generative capability is independent of the physical length scale of the structure. While predictive models can forecast material properties at both the micro – and macro-scale, generative models typically focus on unit cell creation [161,162]. In a multi-scale design, the scaling ratio must be selected considering the printing resolution of the chosen MMAM technique. It remains as the designer’s choice on whether the complexity of multi-material should occur at inter – or intra – unit cell level. Nevertheless, connectivity issues must be addressed when diverse unit cell topologies are present. Functional grading, which demands spatially varying designs tailored to local performance requirements, presents a significant challenge beyond the use of periodically tessellated unit cells. Future research is needed to address this complexity, particularly in integrating inverse-designed unit cells with global optimisation frameworks.

3. Overview of multi-material additive manufacturing processes

AM is a general term referring to the processes of joining materials to make object defined from 3D digital geometry data, usually layer-by-layer. As shown in Figure 11, ASTM

Table 4. Material types in each MMAM process and the capabilities in extending beyond inter-layer planar deposition with discrete material boundaries.

Process	Material	Continuous composition	Intra-layer	Non-planar
PBF	Polymers, Metal	✓	✓	
DED	Metal, Ceramics	✓	✓	✓
Sheet Lamination	Polymers, Composites, Metals			
BJT	Metals, Ceramics			
Material Extrusion	Polymers, Composites	✓	✓	✓
Material Jetting	Polymers	✓	✓	✓
VP	Polymers			

(American Society for Testing and Materials) identified seven main forms of AM to be powder bed fusion (PBF), directed energy deposition (DED), sheet lamination, binder jetting (BJT), material extrusion, material jetting, and vat photopolymerisation (VP). [184].

All these processes began as single-material planar layer-wise deposition. However, significant research into processes have progressed these towards multi-material deposition, or towards advanced geometric capabilities (e.g. non-planar layers), as summarised in Table 4. The transition from single-material to multi-material AM has broadened the scope of AM by enabling fabrication of complex geometries with localised material properties, and multifunctional capabilities.

3.1. Powder bed fusion

PBF is an additive process that enables the creation of high-resolution metal parts. The process begins with a

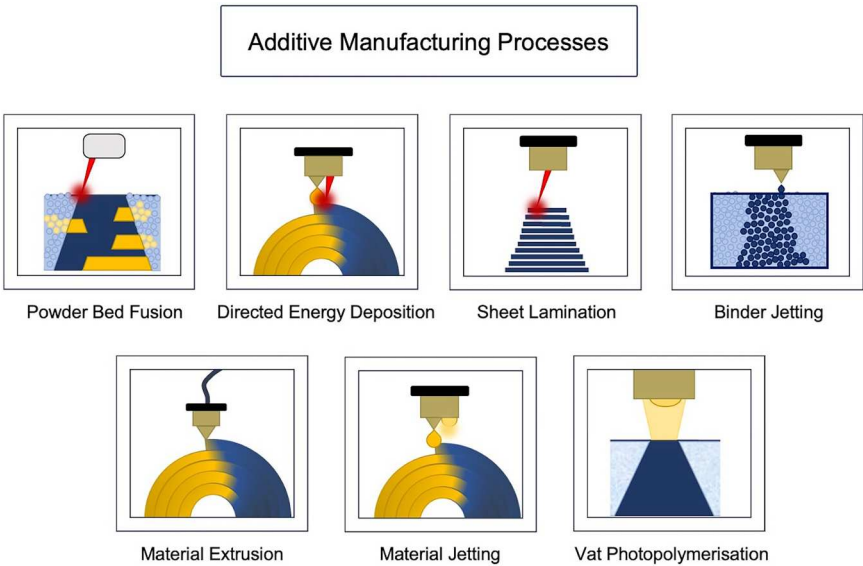


Figure 11. Seven categories of AM as defined by ASTM.

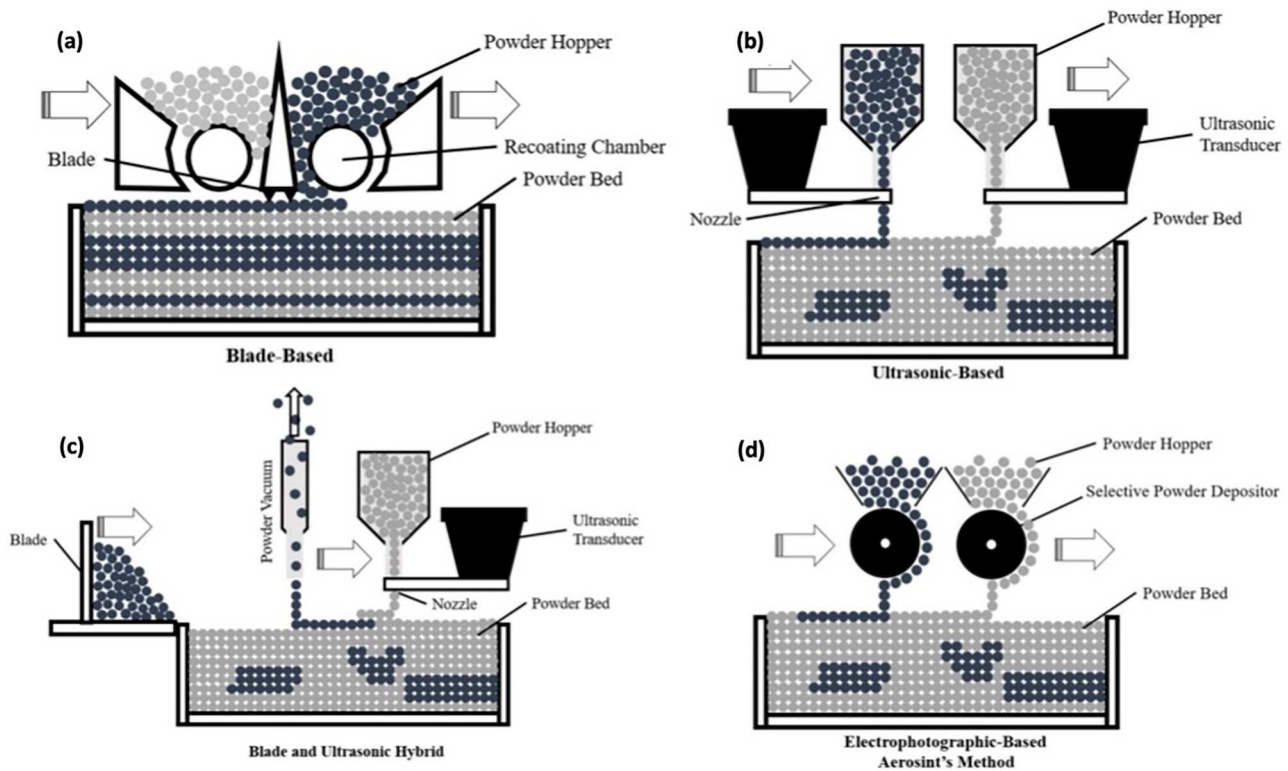


Figure 12. Four methods of selective powder deposition for powder bed fusion: (a) blade-based. (b) ultrasonic-based. (c) hybrid of blade and ultrasonic. (d) electrophotographic-based. Adapted from [16].

thin layer of metal powder being evenly spread across a build platform. A high-powered laser or electron beam then selectively scans and melts the powder according to a digital 3D model, fusing the particles together to form a solid layer. The heat source parameters, such as power, scan speed, and spot size, play a significant role in determining the quality of the melt pool and the resulting microstructure of the part. This layer-by-layer approach is repeated, with the build platform lowering incrementally after each layer is completed, until the entire part is formed.

The primary mechanical challenge in progressing laser powder bed fusion (LPBF) towards multi-material printing is the control of multiple powder materials within the same build environment. This requires advanced powder handling systems that can switch between different powders without cross-contamination. Initial attempts to print with multiple powders including inducing print pauses to allow machinists to manually change the feed-stock mid-print, allowing for inter-layer deposition. However, inherent design limitations are then imposed to only allow for the change of material along the build direction. Techniques such as dual-feed systems and segmented recoaters have been developed to address this issue, allowing for the deposition of different materials in specific regions of the build, proving intra-layer deposition. Four key

techniques have been developed to provide multi-material LPBF, and their recoating systems are demonstrated in Figure 12.

Blade-based: Two recoating blades are used to selectively deposit layers of powder onto a build platform. Each blade can spread a layer of one powder, thus, restricting the change of material along the build direction only. Nadimpalli et al. [185] modified a commercial single blade-based machine to use two powder containers. Their bimetallic builds provided sharp material changes along the build direction only and found that these interfaces were prone to delamination.

Ultrasonic-Based: Ultrasonic-based deposition utilised ultrasonic vibrations generated through a piezoelectric magnetostriction oscillator. These vibrations excite the powder from the hopper and onto the build platform with a resolution in the centimetre scale. This method is capable of depositing multiple materials within a single layer as well as depositing different types of powder at a single location. As a result, it achieves a functionally graded component with non-discrete material boundaries. The primary use-case of this method of powder deposition for LPBF was developed by the Chueh et al. [186], who demonstrated its use to create 3D geometric patterns. Limitations of this method include the efficiency in feeding speed, and the uniformity of the powder layer thickness.

Blade + Ultrasonic Hybrid: This hybrid approach combines the layer-wise deposition of the blade-based method with the intra-layer control of the ultrasonic-based method. The blade is used to deposit the gross material part allotment. The primary material is then selectively melted, and a micro-vacuum removes excess material in unmelted regions. The ultrasonic exciter is used to deposit the secondary material, which occupies a much smaller relative volume.

Electrophotographic-Based: This method uses three powder drums wrapped with a sieve. A vacuum is maintained inside the drum such that the powder is held onto the circumference sieves. As the deposition system moves across the build plate, the drums roll along its surface. A row of piezoelectric valves opens to blow positive pressure against the inside of the sieve to push the powder off the sieve, and onto the build plate below. This allows for the extremely precise (micron-scale) deposition of powder both within a single layer, and across multiple layers.

3.2. Directed energy deposition

Feedstock, either in powder or wire form, is deposited into a substrate using a high-power-density energy source, such as a laser or wire arc. The feedstock is continually fed through nozzles into the melt pool to build material layer-by-layer. The nozzle and heat source are typically mounted on a robotic arm that deposits onto a fixed substrate, or a 1-axis tool head that approaches a 4-axis vice holding the substrate. Since DED feeds material as it builds, the feedstock can be changed mid-deposition to discretely change or grade materials during fabrication. Therefore, the number of materials in a single build is limited by the number of powder feeders or wire nozzles built into the machine. The transition can be achieved through manual or automated processes. Quality of as-printed parts are commonly evaluated for defects (porosity, cracking), and mechanical performance (thermally induced residual stresses, anisotropy) [187].

Unlike most other AM techniques, the 5-axis degrees of freedom allows for the nozzles to deposit onto planar and non-planar substrates. Since the resolution is relatively low due to the larger laser spot size, DED machines are usually combined with a subtractive computer numerical control (CNC) machine to produce a hybrid AM set-up. In this configuration, the machine can pause additive deposition to substantively machine excess material to achieve near-net shape geometry.

3.3. Sheet lamination

The sheet lamination process uses thin sheets of material which are stacked and bonded together,

using either spot welding or adhesive, to form a 3D solid part. After layer-bonding, a laser or cutting knife calibrated to cut to the depth of one sheet layer cuts the 2D cross sectional image based on slice information [188,189]. By alternating the sheet feedstock between layers, a multi-material planar, inter-layer part can be fabricated [188]. Feedstock material is limited to any material that can be rolled sliced into sheets, which commonly includes paper, polymers, and metals, each requiring their own method of adhesion. For instance, metals might be joined using welding processes. Limited studies have examined sheet lamination in a multi-material capacity, due to its limited application space and extreme anisotropy. Mohammadzadeh et al. [190] combined sheet lamination with xurography to create multi-material multilayer microfluidic devices.

3.4. Binder jetting

BJT involves depositing a liquid binding agent onto a powder bed, layer by layer, to form a bonded part geometry. The binder acts as an adhesive by fusing particles together to create a 'green' form, which is sintered to remove the powder binder to achieve a solid, dense part. The method of applying heat after the green part is formed as a final near-net shape part avoids thermal build up and distortion issues seen in LPBF and DED, which often cause geometrical resolution errors, or delamination.

This process is compatible with numerous powdered materials, including metals, sand, and ceramics. While selective powder depositions methods seen in LPBF are theoretically achievable with BJT, they have not yet been commercially developed for this process. Since each powder requires material-specific binder, a method of selective powder deposition for BJT must be developed in conjunction with a means to regionally deposit binder. Commercial machines have been developed to create coloured models by using binders of different colours across a monolithic powder bed. Multi-material BJT has seen an additional process limitation in identifying material pair which provide an appropriate sintering temperature range for both materials to achieve an acceptable densification [191].

3.5. Material extrusion

Material extrusion creates objects by depositing melted material, usually polymers, through a heated extrusion nozzle along a pre-determined path. Controlled pressure is applied to force the material through the nozzle. The material is extruded onto a build platform, or on top of previously deposited layers, and rapidly solidifies to

form a three-dimensional object. The nozzle can be mounted on a planar gantry, as seen in most commercial systems, or on a conformal multi-axis robot arm to provide conformal non-planar printing [192]. The process's feedstock, usually in a filament or pellet form, is loaded towards the hot end of the nozzle. This process is relatively simple, and inexpensive to implement, and has been widely adopted by both industry and hobbyists for rapid prototyping and manufacturing.

Material extrusion has commonly evolved towards MMAM by incorporating multiple nozzles within a single build volume, or by installing a mechanism to automatically load and unload filament from the extruder. The latter method can typically accommodate more materials within a single build but also requires a purge of old material to be pushed out of the nozzle with each material change and can lead to larger feedstock waste.

Material extrusion is limited to thermoplastics, and metals in the case of fused filament fabrication (FFF). Thermoplastics are commonly reinforced using simultaneous thermoplastic and continuous fibre deposition. Composite reinforcement in multi-material extrusion has been shown to significantly improve the mechanical performance of single-material 3D printed plastic [193]. The VF of fibre within the matrix can be adjusted in-situ to optimise the balance between strength and weight. Higher fibre content generally increases strength and stiffness but can also make the material more brittle [194,195]. In continuous fibre reinforcement, the direction of the fibres can be aligned with the principal stress directions, which maximises the load-bearing capacity of the part. This is particularly useful in applications where parts are subjected to directional loads.

3.6. Material jetting

Material jetting operates similarly to 2D inkjet printing, wherein, a printhead dispenses droplets of a photosensitive material onto a build platform. These droplets are solidified layer-by-layer on a planar basis via ultraviolet (UV) light to build a 3D object. While droplet size varies according to the system and material, they are generally in the range of tens of micron in diameter [196], allowing for high-resolution and smooth surface finishes. Material jetting was the first AM technology to enable MMAM by changing the liquid feedstock being deposited. This process is limited to photopolymers and planar layer deposition but can allow for intra-layer multi-material deposition.

Extensive multi-material research has been published using commercial material jetting machines, commonly

PolyJet3D [197–201], ProJet [202], and Connex3 Objet260 [199,200]. Custom-made printers are less prevalent, such as the MultiFab developed by Sittith-Amorn et al. [203,204] which is able to simultaneously manufacture up to ten materials.

3.7. Vat photopolymerisation

VP is a process that fabricates objects by curing a liquid photopolymer resin using UV curable light. The process begins by lowering the build platform into the resin vat. The UV light source (typically a laser or projector) then selectively cures the resin according to the desired pattern of the object's cross-section. The curing process solidifies the resin, and the build platform moves upward one-layer height for the next layer to be cured on top of the previous. This process is known for its high resolution and smooth surface finish, making it suitable for detailed parts of complex geometries.

However, VP is largely limited to single material AM due to the homogeneity of the resin vat. Manual breaks can be made to interrupt the printing process for changing the resin vat to allow for inter-layer MMAM [19], but this process has not yet been automated. Besides increased labour and manufacturing time, another challenge associated with vat change is to manage cross-contamination between liquid resins. While this method provides great dimensional accuracy, its multi-material implementation is also limited by production time, material waste, and the limited material choice of photopolymers.

4. Applications

Recent advances in computational design methods and manufacturing techniques are rapidly expanding the application-space of MMAM, offering new capabilities in both geometric complexity and material allocation. These developments are driving innovation across industries including aerospace [1], energy system [205], electronics [206], soft robotics [207], biomedical [2], and pharmaceuticals [208] (Figure 13). Computational optimisation leverages the design freedom offered by MMAM, enabling functional gradation and regional property tailoring.

Within the aerospace sector, MMAM enables the co-design of structural and thermal performance, where material selection must be tailored to meet specific application needs. Gradl et al. [214] demonstrated that a copper alloy liner, known for its superior thermal conductivity, can efficiently dissipate heat during combustion, while the nickel alloy jacket provides necessary

mechanical strength to withstand high pressures encountered during rocket launches and operation. Similarly, Carroll et al. [215] investigated a stainless steel – IN625 bimetallic combination fabricated through DED for aerospace components such as turbine blades. They argued that this pairing combines the excellent mechanical strength from the stainless steel, with the high-temperature strength and corrosive resistance from the nickel-based alloy. Ren et al. [216] graded Ti-6Al-4 V into Ti-6.5Al-3.5Mo-1.5Zr-0.3Si using DED, targeting compressor blisk applications. They highlighted titanium's strength at room temperature, coupled with its high temperature performance and low thermal expansion coefficient, making it ideal for parts that must maintain structural integrity under varying thermal conditions.

All these multifunctional potentials arise from the diverse properties offered by multiple materials – capabilities that are unattainable with any single material alone.

Electronic and soft robotics sectors have also been advanced by integrating computational design with MMAM techniques. Hou et al. [211] applied design strategies to embed conductive copper tracks within flexible polyethylene structures using LPBF, enabling complex, multi-layered 3D circuits (Figure 13c). In soft robotics, Zolfagharian et al. [217] applied the MM-SIMP method to design polyelectrolyte actuators fabricated via material extrusion. By distributing materials according to local stress fields, they enhanced actuator performance by leveraging the stimulus-responsive nature of hydrogels. Likewise, Sundaram et al. [218] leveraged

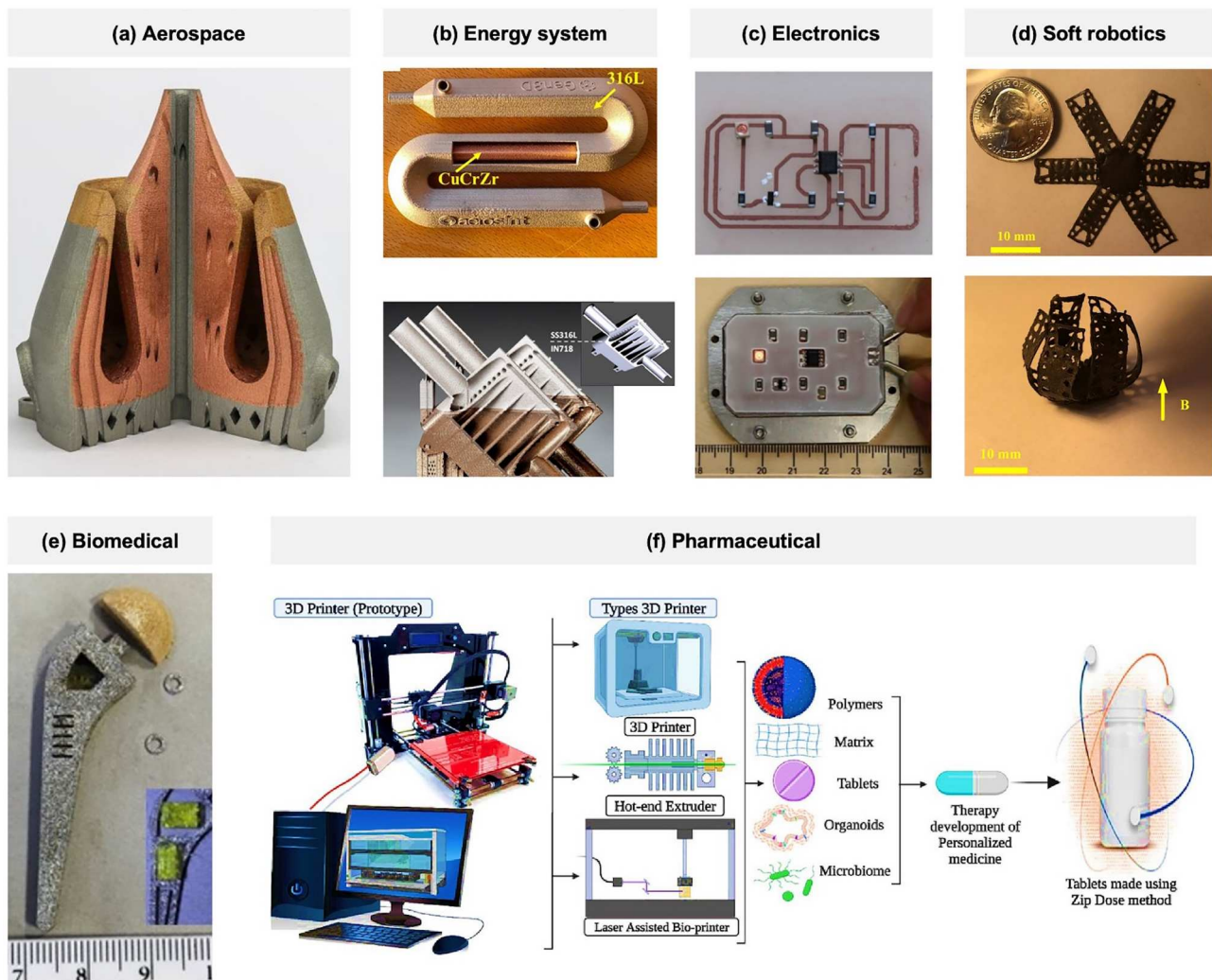


Figure 13. MMAM design applications. (a) Multi-material 'Aerospike' rocket nozzle fabricated by MM-LPBF, reprinted from [209] with permission from Aerosint. (b) Multi-material heat exchangers, reprinted from [16] and [210] with permission from Taylor & Francis and Elsevier, respectively. (c) 3D multi-layered circuit, reprinted from [211] with permission from Elsevier. (d) 4D printing of a flytrap soft active structure, showcasing the shape change in response to magnetic field. Reprinted from [119] with permission from Elsevier. (e) Multi-material hip implant with bio-degradable polymer embedded inside the metal structure, reprinted from [212] with permission from Elsevier. (f) Active pharmaceutical ingredients and excipients in multi-material 3D printed tablets. Reprinted from [213] with permission from Elsevier.

the voxel-level deposition precision offered by multi-material jetting to fabricate soft robotic actuators. By combining soft and rigid acrylate polymers with a magnetic nanoparticle polymer composite, they simultaneously optimised the actuator's geometry and its deformation behaviour under an applied magnetic field using simulated annealing strategy.

Computational design has become especially critical in emerging pharmaceutical manufacturing applications. A review by Liu et al. [208] discusses the emergence of ML and physics-based modelling to optimise the spatial distribution of active pharmaceutical ingredients (APIs) and excipients in multi-material 3D printed tablets. This approach allowed precise control over drug release profiles, improving therapeutic outcomes while meeting scalability and regulatory standards. Recent advances in polymer science, computational validation (e.g. CNN-based quality control), and hospital-based implementation guidelines [219,220] have accelerated clinical deployment of MMAM in pharmaceutical applications.

Despite the growing availability of computational design tools, multi-material applications remain in the early stage of development for commercial utilisation. Only a small number of computationally optimised designs are physically fabricated, primarily for prototyping purposes instead of experimental verification. MMAM fabrication facilities are still largely confined to research settings and have yet to see widespread adoption in industry. However, MMAM has the transformative potential to revolutionise critical industries as research progress, driving innovation and redefining design possibilities.

5. Research challenges and opportunities

Despite the growing development of MMAM design methods, discrepancy still exists between computationally-optimised results and manufactured products. The discrepancy can arise from assumptions in modelling, such as perfectly bonded multi-material interface and simplified material responses. The discrepancy can also stem from simplifying or neglecting

manufacturing constraints, inadequately capturing material strength and failure criteria, or ignoring uncertainties in fabrication and operational stages. Section 5 reviews state-of-the-art implementations to address above-mentioned challenges, where strategies were sometimes shared across diverse design methods (Table 5). Future research directions are suggested to facilitate the adoption of multi-material applications across sectors.

5.1. Multi-Material interface

5.1.1. Experimental characterisation of interfacial properties and defects

Interfacial properties are typically characterised by tensile or flexural strength, with the interface plane oriented either laterally or longitudinally to the loading direction. However, the absence of dedicated MMAM testing standards (i.e. specimen geometry, process parameters and testing conditions) has led most researchers to adopt those developed for single-material AM. Lateral tensile testing remains the most common approach to evaluate interfacial strength across metals [260,261], polymers [262,263], and hybrid systems [264]. Efforts to enhance interfacial bonding have included tuning processing parameters – such as increasing nozzle temperature [265] or adjusting extrusion speed [266] – and redesigning interface geometry through mechanical interlocks [267] or surface textures [268]. These physical enhancements, however, are rarely captured in computational design due to their reliance on localised process physics or high-resolution geometrical features, highlighting a limitation in current modelling frameworks.

Failures in multi-material components can occur either at the interface or within the bulk material, depending on processing conditions and material compatibility factors. In the cases where strong metallurgical bonding formed, bimetallic tensile specimens outperformed the weakest bulk material [269,270]. However, due to material discontinuity and a general uptake in local defects, failure at the interface is also commonly reported [261,271]. Cracks, pores [271], and irregular

Table 5. State-of-the-art in addressing MMAM research challenges by different MMTO methods.

		Density-based	Evolutionary	Level set	Phase field	AAP
5.1	Multi-material interface modelling and control	[221–226]	[87]	[227–231]		
5.2	Advanced material response modelling (anisotropy, beyond linear elasticity)	[232–235,302,303,238–240]	[82,241]			[141]
5.3	Manufacturability (LSC, dimensional and assembly constraints)	[242–245]	[88]	[121,246,122]		[141]
5.4	Material strength and failure criteria	[56,247,235,248–252]	[77,81,82,87]	[105,106,253,254]		[138]
5.5	Robustness under uncertainty	[59,255–259]	[86]	[230]	[127]	[140]

formation of intermetallic phases [272] have been observed at dissimilar metal interfaces, compromising bond quality. Vertical interfaces in intra-layer design are more prone to defect formation due to composition-dependent laser processing parameters [273]. Failure away from interfaces is the goal of interfacial bond strengthening studies. Recognised contributing factors, many of which are not yet fully understood, include material capability in solubility, thermal conduction, thermal expansion, refraction, and solidus temperature. Relevant processing conditions may include localised interfacial parameters, or the possibly of post-processing heat treatments to remove the formation of defects [272,274].

To inform computational design, accurate characterisation of interfacial properties is essential. Experimental insights are therefore required to develop more realistic interpolation schemes. Numerous studies, across multiple MMAM processes (e.g. LPBF [261,275–279], DED [280–285], material jetting [199]), have revealed micron-scale transition zones at discrete interfaces, typically marked by grain refinement, porosity, cracking, and heterogeneous hardness. Indentation-based hardness testing is frequently used across metal interfaces to map gradients in material properties across boundaries. Techniques such as the Oliver and Pharr method [286] can also extract local Young's modulus or yield strength. Conversely, polymeric and hybrid material interfaces are more often assessed via tensile pull-apart tests to quantify interfacial bonding strength. Overall, these experimental measurements inform the assignment of interfacial properties in computational design frameworks.

Gradual transitions in hardness across metallic interfaces are commonly observed, particularly in steel/copper – [261,275,279] and steel/nickel-based alloy pairs [271,287–291]. Similar trends have also been reported, though less frequently, for titanium/nickel – [292], nickel/copper – [293], and titanium/aluminium-based alloys [294]. Alternatively, for some material combinations, the interfacial region can be characterised by a regional increase in hardness due to potential grain refinement or the formation of secondary and intermetallic phases [295,296]. The formation of grain refinement is known to hinder grain dislocation, leading to an increase in local hardness. Nevertheless, the ability to tailor interfacial mechanical properties through process parameters remains largely underexplored from an experimental perspective [284]. This underscores the need for computational design frameworks with the flexibility to represent interfaces as either discrete or graded regions, enabling accurate modelling of interfacial properties to reflect material or process conditions.

5.1.2. Interface representation, modelling and control

Computational design methods typically represent multi-material interfaces as discrete boundaries with abrupt property transition and perfect bonding assumptions. To better reflect experimental observations, emerging approaches instead represent interfaces as graded regions, enabling more nuanced control over interfacial properties. In density-based MMTO, Chu et al. [221] have successfully controlled the width of the interface zone by adopting an extended two-step filtering approach consisting of density smoothing and projection scheme, originally used in coated structure design [222]. A large norm of spatial gradient was added to the MM-SIMP scheme to interpolate interfacial properties. Tajs-Zielińska et al. [223] introduced an efficient heuristic topology generator, known as the Cellular Automata approach, to optimise graded multi-material structures. Lin et al. [224] performed multi-scale optimisation of multi-material structures with non-periodic infill, highlighting that interface stiffness at the microscale could be enhanced by considering strain gradient.

Graded-interface-representations were also investigated under the boundary-controlled design, especially within the CLS and MMLS methods. Both monotonic and non-monotonic property variations over the interface zone were explored [228]. In the latter case, the interfacial properties were not restricted within the range of the neighbouring bulk properties, providing the flexibility to model strong or weak interfaces according to the experimental observations [229] (Figure 14). The stochastic response raised from uncertainty in a graded interface was formulated as a random field and then predicted by the Polynomial Chaos expansion method by Kang et al. [230]. Case studies were conducted for composites with extreme thermoelastic properties, revealing that interpolating for the interfacial zone did affect the optimisation result [231]. It is also worth noting that discrete representation can introduce sensitivity issues in shape derivative evaluation, whereas graded interfaces help facilitate convergence [227].

Accurate modelling of interface behaviour remains critical for further advancing MMAM. Computational-design-oriented studies often rely on normalised elastic modulus to demonstrate the feasibility of proposed methodologies. Prospective studies should integrate experimental findings – such as microhardness testing, interfacial strength measurements – into the design framework. These data can inform the development of more realistic interpolation functions that capture the non-linear and often asymmetric behaviour at multi-material interfaces. Further investigation should also focus on multi-physics coupling to capture the

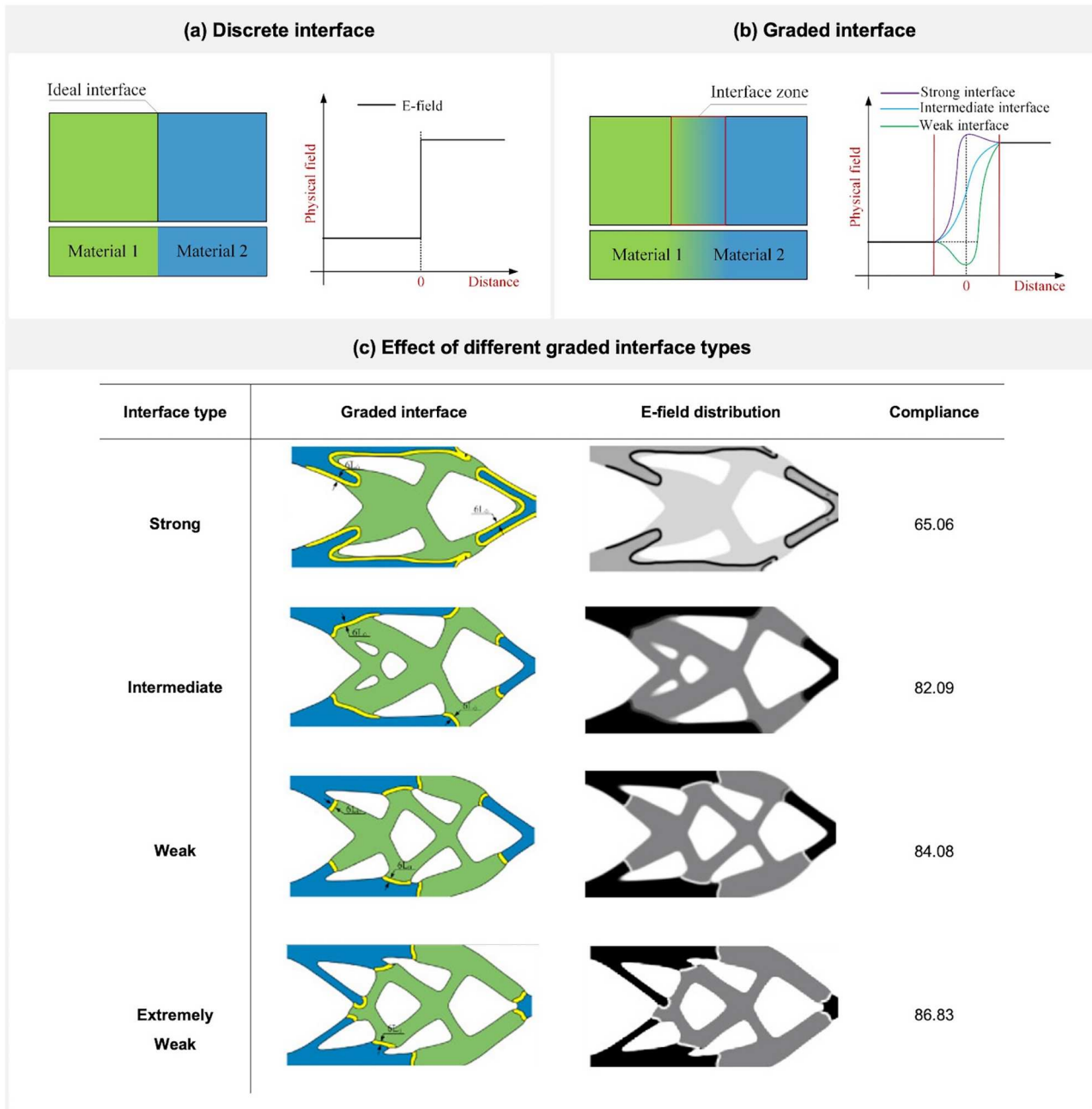


Figure 14. Multi-material interface modelling. (a) Discrete interface with a sharp transition in the physical field. (b) Graded interface zone, in which the interfacial property could be higher / intermediate / weaker than the neighbouring materials (c) Compliance minimisation of a three-phase cantilever beam considering different interface types with a fixed interface width. Reprinted from [229] with permission from Elsevier.

interplay between heat transfer [297–299], phase evolution, and mechanical fracture [300,301] at the interface. Incorporating interfacial delamination and fracture through cohesive zone modelling or extended finite element methods (XFEM) offers promising avenues [302]. Ongoing research into interfacial responses under complex loading, such as contact [303] and impact [304,305], remain confined to simulation studies and have yet to be integrated into optimisation frameworks.

While interface modelling has received growing research attention, interface control strategies are still in infancy. Future work is required to develop regularisation techniques that penalise unfavoured material combination based on compatibility metrics, or penalise interfaces subjected to unfavoured loading conditions. To remark frontier research in this aspect, Shah et al. [225] proposed a pseudo-cost domain method that evaluates the relative joining cost of different material pairs. Considerations such as material compatibility,

manufacturing feasibility, joint property and reliability could be indirectly integrated, consequently penalising unfavoured material combinations. Similarly, Kim et al. [226] introduced interfacial tension energy density into the objective function, such that interfacial regions subjected to tensile stress are restricted. Building upon these early advances, the integration of interface regularisation mechanisms into full-scale computational design frameworks will be critical to achieving reliable and manufacturable multi-material solutions.

5.2. Material response modelling

5.2.1. Anisotropy

Reducing anisotropy caused by layer-wise deposition has been the focus of many metal AM studies. Homogeneity of the microstructure can be driven by material choice [306] and processing parameters such as deposition rate [307], build environment [308], and laser scanning strategy [309–311]. Post-processing heat treatments have proven effective in mitigating anisotropy by homogenising microstructure and redistributing residual stresses [312–314]. However, extending such strategies to MMAM is challenging due to material incompatibility, particularly the need for overlapping heat treatment temperature windows [272], [274]. Deposition-induced anisotropy remains a practical challenge but is often neglected in computational design, which commonly assumes idealised isotropic material behaviour.

Given the challenges in overcoming anisotropy within multi-material parts through processing or post-processing conditions, computational design tools have instead evolved to consider directional anisotropic material behaviour. Solid Anisotropic Material Penalisation (SAMP) modified the interpolation scheme in SIMP by replacing Young's moduli with constitutive tensors. Similarly, Eckrich et al. [241] adopted anisotropic BESO to optimise part shape and fibre orientation, while the fibre placement paths were further derived based on the stress state. Although directional dependency has been addressed, asymmetry of yield strength under tensile and compressive loads still lacks research attention. Liu et al. [247] computed a safety factor based on the Tsai-Wu yield criterion, then formulated the strength-based TO problem as minimising the max failure index under total mass constraint (i.e. min-max problem).

Still, neither SIMP nor SAMP can simultaneously optimise multi-material structures consisting of both isotropic and anisotropic materials. One industrial example would be the passenger aircraft seat [232], where anisotropic composites were utilised to replace isotropic

metals at non-load-bearing regions for weight-saving. Since the applicability issue arises from the material interpolation, Li et al. [233] proposed an element interpolation scheme, in which the property at each voxel is represented as a weighted sum of coincident single-material finite elements. Bohrer et al. [234] later claimed that the element stacking process involved will lead to computational burden during FE analysis, consequently proposing a coupled material interpolation method similar to DMO, but offering an alternative for sensitivities calculation. The stress-constrained MMTO framework proposed by Kundu et al. [235] allows the optimisation of fibre orientation in the anisotropic material phase. It is revealed that anisotropic materials are favoured in uniaxial members for stiffness enhancement, whereas isotropic materials are essential at multi-axially stressed joints to improve strength (Figure 15).

While studies have started to optimise printing orientation when anisotropic materials are involved, process-induced anisotropy is still largely overlooked. Recent work on tool path planning, such as Weeks et al.'s investigation [315] into the effects of ink rheology and print paths on mechanical performance of multi-material polymer lattices, highlights the need for tighter integration between part design and process planning. Advancing this linkage could enable more accurate predictions of anisotropic behaviour and ultimately lead to more reliable and tailored multi-material components.

5.2.2. Beyond linear elasticity

Most existing studies in MMTO rely on linear elastic material assumptions for computational simplicity. However, nonlinearity or inelastic responses are commonly observed in practical engineering applications. For metals, elastoplastic models are essential to account for strain hardening, while rubber-like materials require hyperelastic models to handle large, reversible deformations. Concrete, with its distinct moduli in tension and compression, also necessitates bimodular modelling.

Key challenges in integrating multiple nonlinear elastic materials into MMTO have been identified by Zhang et al. [236,237], which are material interpolation, excessive distortion in low-density elements, and high computational cost. To address these, a DMO-type interpolation scheme was introduced to handle multiple stored-energy functions flexibly. Since nonlinear material behaviour requires solving nonlinear state equations, adaptive mesh refinement was incorporated to manage computational load effectively. Additionally, the ZPR update scheme [238] was adapted, allowing independent updates of design variables under multiple volume constraints. This framework has been further extended to optimise hyperelastic structures with

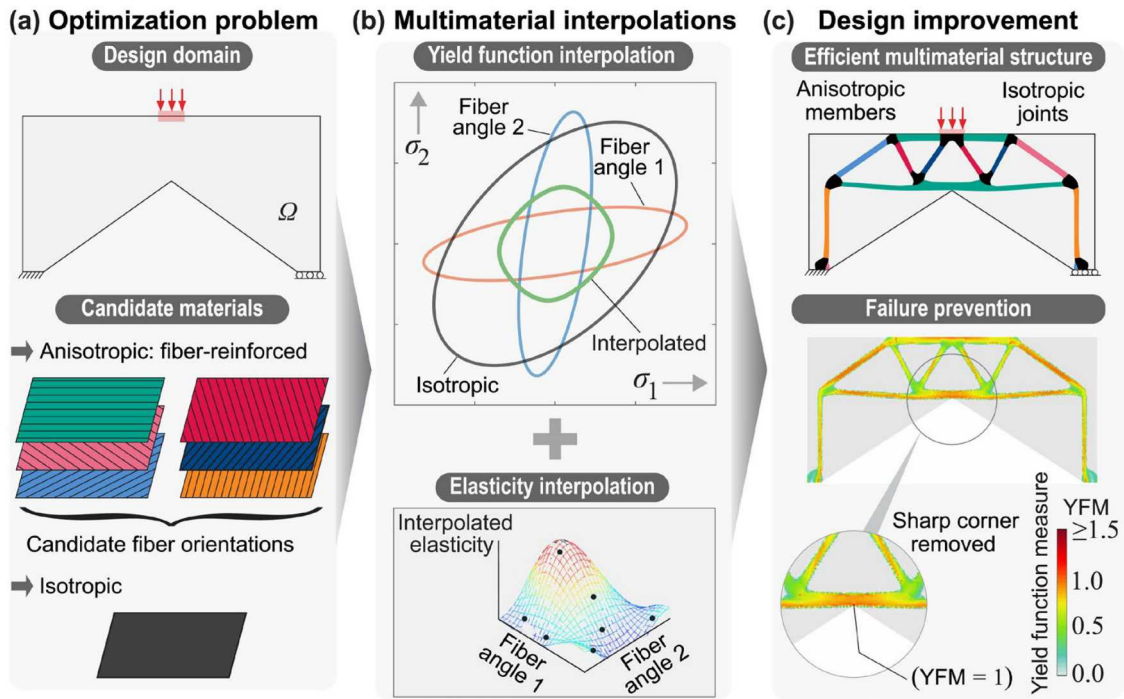


Figure 15. The stress-constrained MMTO framework proposed in [235], integrating anisotropic fibre-reinforcement and isotropic materials. (a) Optimising fibre-reinforced composite. (b) Multi-material interpolation schemes related to the yield function and elasticity. (c) Local stress concentration was effectively reduced with the optimised configuration, which consists of anisotropic members and isotropic joints. Reprinted from [235] with permission from Elsevier.

anisotropic fibre reinforcement under large deformations [239].

Elastoplastic models are critical for capturing irreversible deformations and energy dissipation under extreme loading. Jia et al. [240] conducted multi-objective optimisation of composite structures to achieve target elastoplastic responses, including enhanced initial stiffness, delayed plastic yielding and maximised energy absorption (Figure 16). Different hardening rules are handled by the return mapping algorithm supported by the plasticity theory. It is revealed that sequential yielding could be strategically leveraged to prolong post-yielding resistance. Overall, future research in MMTO should move beyond linear elastic assumptions to capture more realistic material responses.

5.3. Manufacturability

MMAM inherits manufacturing constraints in conventional AM processes, such as minimum printing resolution, maximum build size, overhang angle limitation, and support removal considerations. Some processes such as polymer-AM strategically use their multi-material capabilities to deposit dissolvable support material for easy removal, especially for entrapped surfaces [316]. In VP, multi-material capabilities have been exploited by injecting resins through fluidic channels

embedded within the part design, thereby offsetting forces that would otherwise require support [317].

5.3.1. Length scale control

LSC is a computational implementation to ensure design features comply with the fabrication limits of the selected manufacturing processes. In density-based MMTO, Song et al. [242] suggested to manage max LSC by introducing porosity and material rate, while regulating min LSC based on geometric constraints and indication functions with a normalisation gradient norm. Taheri et al. [243] extended the isogeometric approach by imposing perimeter restrictions, allowing control over the rate of transition between material phases within functionally graded materials (FGMs). Beyond designing primary structures, Giraldo-Londoño et al.' work [244] also enabled sequential optimisation of support structures with an overhang angle detection algorithm (Figure 17b). By proposing regional volume constraints, the max feature size of the support is restricted to facilitate removal during the post-processing stage.

In evolutionary MMTO, sequential approximate integer programming was employed to improve the computational efficiency of the min LSC problem [88]. LCS strategy for orthotropic multi-material was investigated by Zhang et al. [141] under the AAP framework

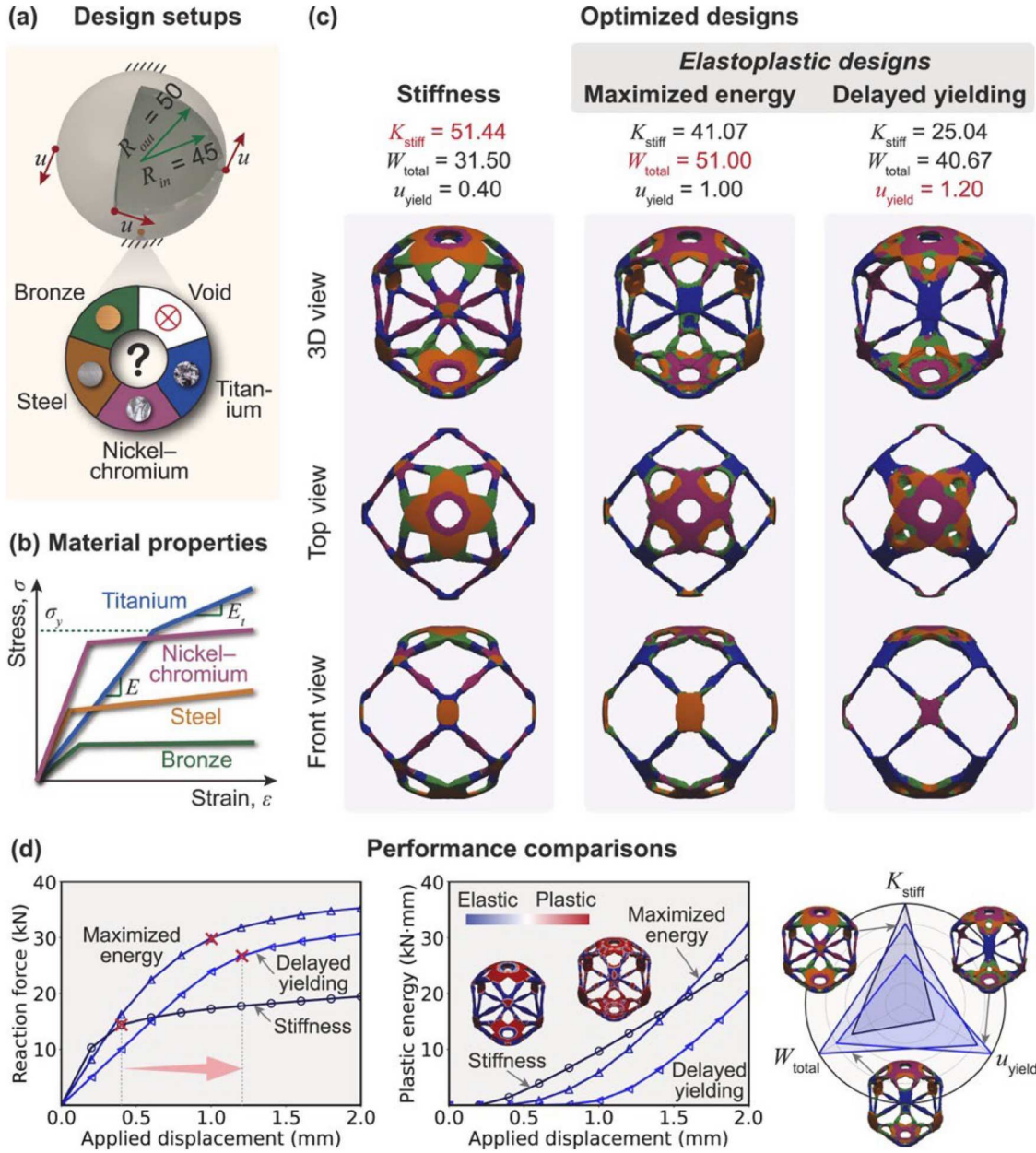


Figure 16. Optimising a three-dimensional multi-alloy elastoplastic structure. (a) Design problem setup. (b) Elastoplastic properties of the solid material candidates. (c) Multi-material designs optimising for initial stiffness (K_{stiff}), total energy (W_{total}) and yield displacement (u_{yield}), respectively. (d) Performance comparisons of three optimised designs. Structural yielding is denoted by the crosses in the force-displacement curve. Reprinted from [240] with permission from Elsevier.

(Figure 17a). Violation against geometric bounds could also be formulated as a soft constraint penalising the objective function, as implemented by Lie et al. [246] in the LS method. In TO formulation with NNs, the length scale filter was approximated by adjusting the frequency band of a Fourier projection layer, eliminating the need for directly imposing constraints [318].

5.3.2. Dimensional and assembly constraint

Large-scale multi-material engineering applications [319] may require separate fabrication of individual

components followed by assembly. As restricted by the maximum build volume of the selected MMAM process, Feng et al. [122] incorporated dimensional limitations into the extended LS method, with a follow-up work [121] simultaneously considering assembly constraints (Figure 18). A sequential optimisation workflow between multi-material and multi-joint was proposed by Florea et al. [245], not only considering the stiffness difference between joint types (e.g. weld vs. adhesive bond) but also the corresponding tooling accessibility. Building on this method, joint cost could further reflect

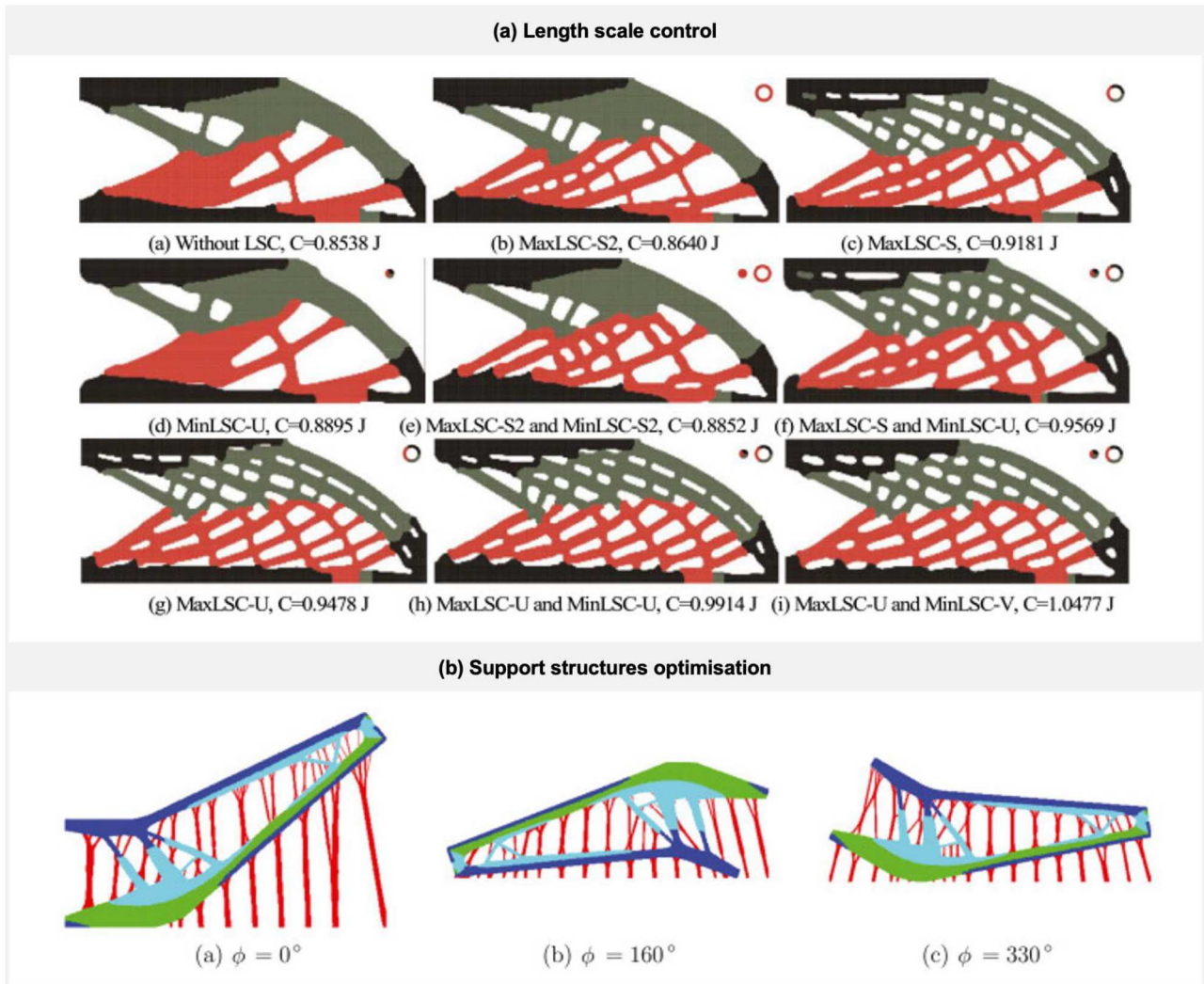


Figure 17. Manufacturability consideration with respect to feature size and support structures. (a) Topology optimisation of a cantilever beam with different max/min LSC schemes applied to each material. Reprinted from [141] with permission from Elsevier. (b) Effect of printing orientation in the optimised topology of a multi-material antenna bracket's support structure. Reprinted from [244] with permission from Elsevier.

material compatibility, enabling penalties for undesirable interfaces between specific material pairs in multi-material designs. Note that these manufacturing considerations for multi-material structures are also applicable to conventional fabrication methods beyond AM.

5.4. Material strength and failure criteria

Stress is a critical failure indicator in structural optimisation, especially at material interfaces where high local stresses can cause delamination or fracture. Traditional compliance-based methods overlook strength limits, prompting, for example, the use of stress-constrained mass minimisation for safer designs. However, stress constraints are difficult to implement due to their non-linearity, localisation, and mesh sensitivity. A common approach is to use an aggregation

function (e.g. p-norm) to enforce a global stress constraint.

In the density-based MMTO framework, a separable stress interpolation (SSI) scheme was developed, which distinguishes the interpolation function between material properties and stress norm evaluation [248]. By adopting element/patch stacking methods, stress constraints were computed for each material candidate, resolving the ill-posed issue where design variables for multiple materials simultaneously converge to full density to satisfy stress constraints [320]. To avoid introducing another set of design variables, Xu et al. [56] proposed an ordered SIMP-like interpolation function for relaxed and scaled stress (Figure 19a). Similarly, Liao et al. [249] developed a stair-form interpolation model suitable for stress-minimisation design involving unstructured meshes.

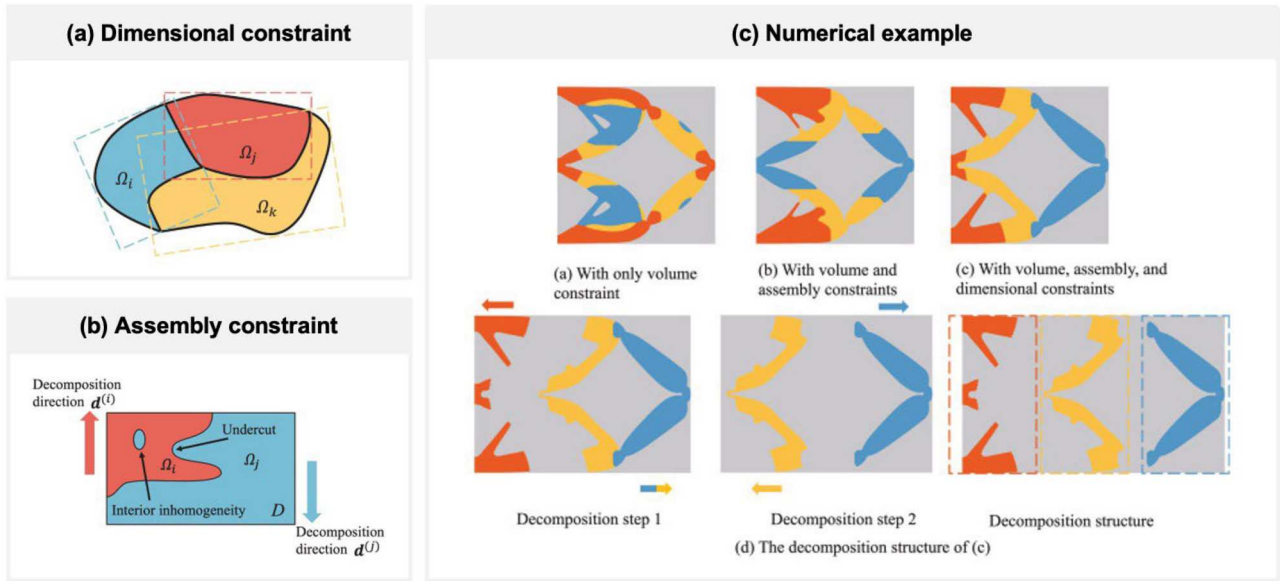


Figure 18. Manufacturability consideration with respect to maximum build volume and assembly process. (a) Bounding boxes of each material component that must be fit within the maximum build volume of a 3D printer. (b) Illustration of the interior inhomogeneity and undercut that prevents multi-material decomposition/assembly (c) A case study showing topological changes after applying assembly and dimensional constraints, as well as the decomposition sequence. Reprinted from [121] with permission from Elsevier.

Kundu et al. [250] proposed a yield function interpolation scheme that considers not only differences in material stiffness and strength, but also distinct yield criteria (e.g. von-Mises for steel rebar; Drucker-Prager criteria for concrete). Hu et al. [251] proposed a tension/compression-asymmetric piecewise interface stress constraint to account for the difference in interfacial strength when more than one materials pair are present. Application wise, Sui et al. [252] demonstrated that incorporating stress constraints effectively reduced stress concentration at the hinge of a multi-material thermo-hyperelastic compliant mechanism.

Stress constraints were also investigated within the context of compliant mechanism design under the MMLS framework. The Augmented Lagrangian method is utilised for introducing stress within the objective function as a soft constraint. The study by Chu et al. [106] considered the maximum stress among all material phases while Emmendoerfer et al. [105] focused on evaluating interfacial stress specifically. Similarly, a quadratic stress criterion consisting of both the shear and normal tensile stresses at a narrow-banded interface was proposed by Liu et al. [253] (Figure 19b). Intersection points found on the LS grid were used to generate body-fitted meshing along the material boundary. Besides, stress-constrained CLS scheme was also examined by performing shape sensitivity analysis under the Eulerian description [254].

Future work on failure-constrained MMAM design should incorporate more comprehensive and material-

specific failure criteria. Beyond yielding, failure mechanisms like delamination, fracture, and buckling should be explicitly modelled. Introducing fracture toughness or energy release rate as constraints within optimisation could improve robustness against cracking. Additionally, residual stresses arising from mismatched thermal expansion coefficients or deposition sequences need to be better integrated into the design process. Finally, future models should address the underestimation of stress concentration effects in homogenised multi-scale frameworks to more accurately capture local failure risks.

5.5. Robustness under uncertainty

Deterministic optimisation, the default approach in reviewed literature, overlooks uncertainties from variable loading conditions, stochastic material properties [321], and geometric discrepancies in printed parts [322]. The width of the graded interface zone and the corresponding property is another source of uncertainty specific to the multi-material design case. It is essential to quantify the sensitivity of the optimisation objective with respect to these variations, incorporating the robustness requirement as early as in the computational design stage.

In probabilistic robust optimisation, design scenarios follow a defined probability distribution (e.g. normal, uniform). The objective function is computed deterministically for each scenario, with the optimisation goal

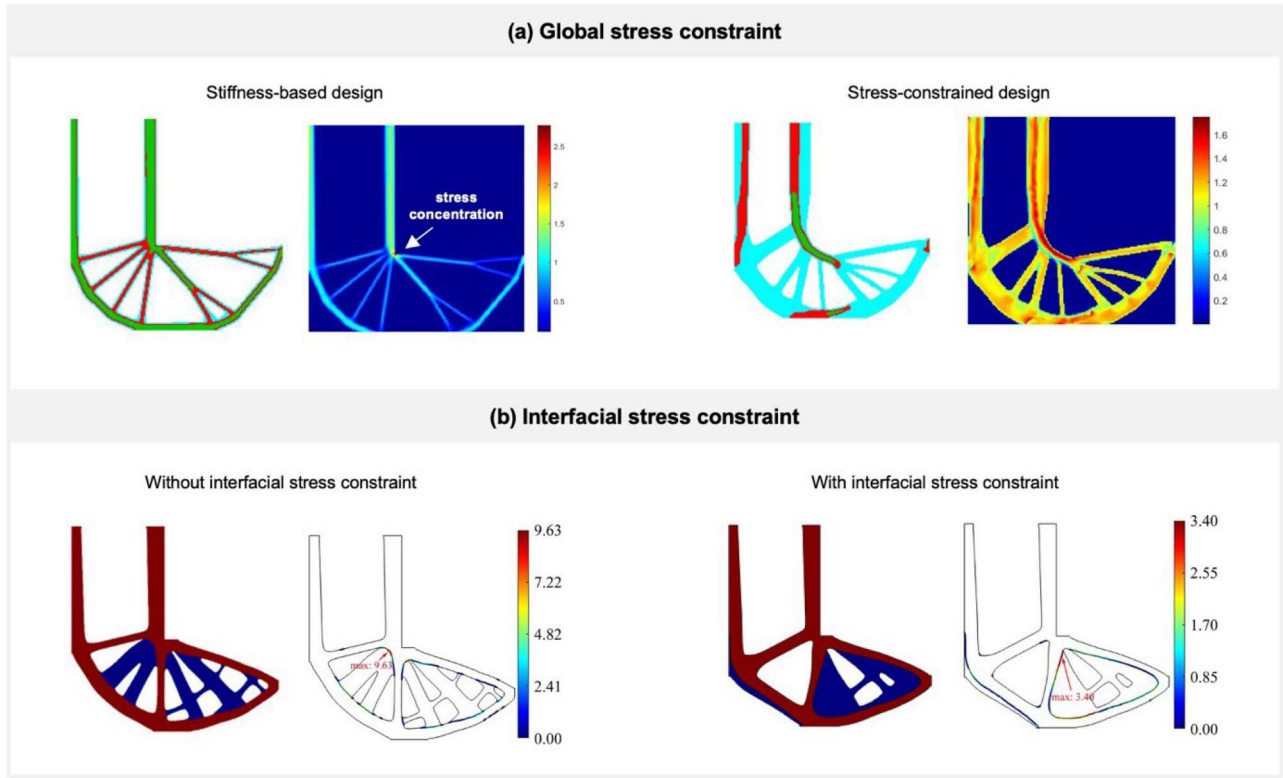


Figure 19. Multi-material design incorporating stress constraints. (A) The design subjected to global von-Mises constraint reduces the stress concentration in the L-shaped bracket compared to stiffness-based solution. Reprinted from [56] with permission from Elsevier. (B) Control over the peak interfacial stress (reduction from 9.63 to 3.40) by enforcing interfacial stress constraints. Reprinted from [253] with permission from Elsevier.

being a weighted sum of the mean and standard deviation, shown in Equation (6).

$$\min_{x \in \mathcal{X}} \left(\sum_{i=1}^N p_i f(x, \xi_i) + \lambda \cdot \sqrt{\sum_{i=1}^N p_i \left(f(x, \xi_i) - \sum_{j=1}^N p_j f(x, \xi_j) \right)^2} \right) \quad (6)$$

where x is the design variables, ξ_i is scenario i with probability p_i such that $\sum p_i = 1$, $f(x, \xi_i)$ is the deterministic evaluation of the objective under scenario ξ_i , λ is a user-defined weight to penalise variability.

The probabilistic model has been incorporated into various MMTO frameworks in response to loading uncertainties (Figure 20), including ordered-SIMP [59], soft-kill BESO [86], and density-based AAP [140]. Techniques such as orthogonal diagonalization of the force vector [140], material field series expansion [255], and sparse grid numerical integration [59] have shown effectiveness in reducing the computational burden of the Monte Carlo simulation. Variation in material property received less research attention compared to loading conditions, with only Kang et al. [256] considering uncertainty in E and ν . Reaction or inter-diffusion between materials results in interface uncertainty. By modelling the

interface zone width with a random Gaussian field, the same research group formulated the robust optimisation problem under both the LS [230] and phase field [127] MMTO framework.

Non-probabilistic reliability-based optimisation is an alternative to ensure the robustness of the design, particularly suited if there is a deficiency in sampling data or a limitation in computational resources. Alacoque et al. [257] addressed the loading uncertainty in optimising thermoelastic multi-material periodic microstructures by considering the worst-case stress state. Cheng et al. [258] constructed an ellipsoidal model to control load uncertainty for a volume minimisation problem with stress constraint. Heat-transfer structures with unknown-but-bounded uncertainties were explored by Wang et al. [259], where non-probabilistic reliability constraints were used to replace deterministic thermal limits.

5.6. Multifunctional: beyond structural role

Optimisation objectives and constraints in multi-material design should be broadened to address growing demands for multifunctional applications. In MMTO (Section 2.1), most methods prioritise stiffness

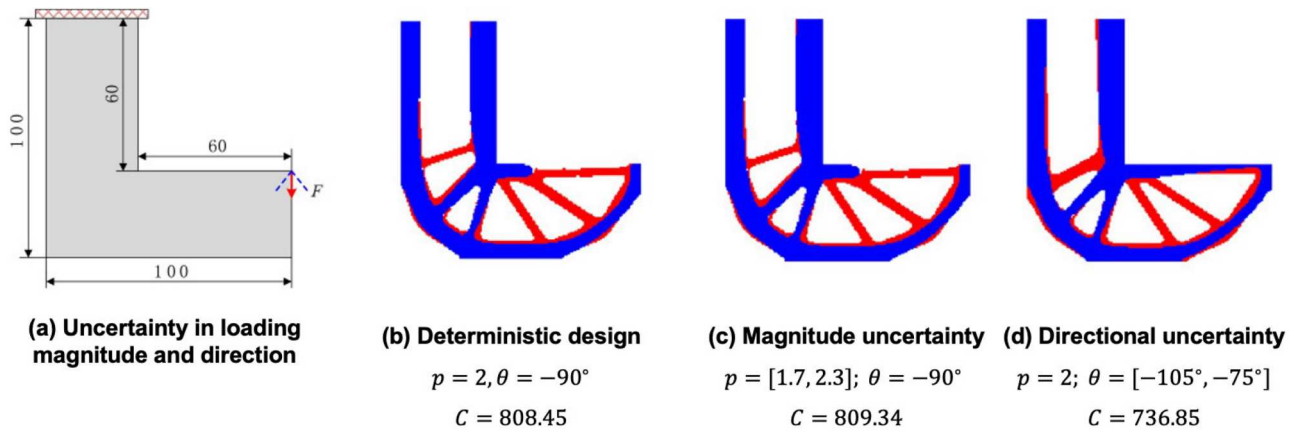


Figure 20. Multi-material design considering uncertainty. (a) Compliance minimisation of a multi-material L-shaped structure using (b) deterministic and (c&d) robust formulation, respectively. Directional uncertainty is observed to have more significant effects on the topological configurations than magnitude uncertainty. Reprinted [86] from with permission from Elsevier.

and weight reduction, with some extending to compliant mechanisms or stress-constrained formulations. ML-based approaches (Section 2.2) focus on tailoring compressive behaviour, Poisson's ratio, or anisotropy in lattice structures. Applications have largely remained in the structural domain (Figure 21a–c), where mechanics is the governing physics. Within this scope, the aerospace sector tends to be objective-driven whereas biomedical applications are often governed by strict constraints.

Nevertheless, the potential of multi-material design extends beyond structural functions to thermal, electromagnetic, and acoustic domains (Figure 21d–g). For instance, combining stainless steel with copper enables thermally efficient, mechanically robust heat exchangers. In soft robotics, integrating stimuli-responsive materials in matrices enables programmable actuation. Advancing multi-physics, multi-objective optimisation will be key to realising such multifunctional applications.

5.7. Toward integrated design-manufacturing-validation

The STL (STereoLithography) format, widely employed in rapid prototyping, represents a 3D object with material-agnostic triangular surface meshes [325]. Current adaptation of STL for MMAM involves individual component exportation and manual material assignment in the slicing software, a process known as homogeneous multi-material design. Advanced formats like AMF (Additive Manufacturing File Format) [326], 3MF (3D Manufacturing Format), and MAMF (Multi-material Additive Manufacturing File) [327] support multi-material data, but remain focused on discrete material compositions.

To enable functional grading, heterogeneous design approaches have emerged using either voxel representations or boundary-surface models [328–332]. However, despite growing capabilities, these advanced file formats have yet to achieve widespread adoption in both research communities and industrial settings.

The lack of experimental validation for multi-material optimisation outcomes is a persistent issue in the AM community. While few studies have experimentally tested multi-material lattice structures, they are generated using control variables instead of optimisation algorithms, with experiments often limited to compressive testing [31,33,333,334]. The gap arises due to the distinct domain expertise required for computational design and manufacturing, with many researchers lacking access to suitable fabrication facilities. Some design methodologies are overly performance-driven, overlooking manufacturing constraints, which makes fabrication impossible from the outset. To ensure fair comparisons across studies, it is suggested to establish numerical benchmarks in the field of computational design (e.g. MBB beam, cantilever beam, two-bar bracket, three-pointed loaded beam, L-shaped structure, etc). Ultimately, bridging the gap between computational design and manufacturing requires increased collaboration across disciplines.

6. Concluding remarks and outlook

This article summarises the state-of-the-art in computational design for additively manufactured multi-material structures, covering both TO methods and data-driven approaches. Guidelines were provided to select computational design tools and manufacturing processes that fulfilling multi-material design aspects.

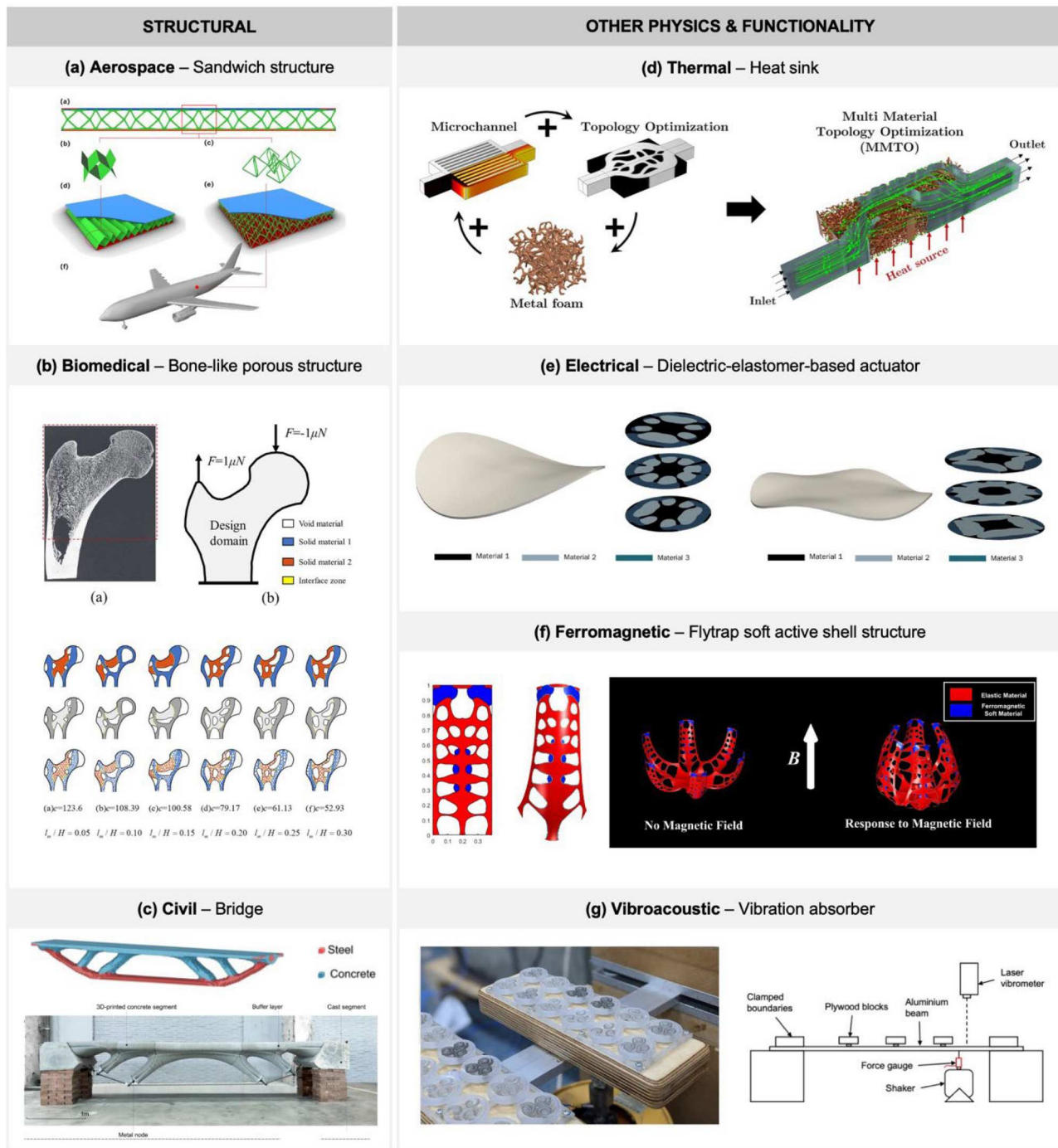


Figure 21. Application of multi-material computational design methods within and beyond structural functionality. (a) A three-material sandwich panel was designed for aviation to resist bending loads, with MM-BESO employed to account for differences in tensile and compressive properties. Reprinted from [82] with permission from Elsevier. (b) A bone-like porous structure that exhibits high impact resistance, effective heat transfer and liquid diffusion. Designed using concurrent cross-scale MMTO algorithm considering interface strain gradient. Reprinted from [224] with permission from Elsevier. (c) A cable-supported, unreinforced 3D-printed concrete bridge designed using MM-BESO. Reprinted from [83] with permission from Elsevier. (d) A microchannel heat sink design obtained from MM-SIMP, in which the distribution of solid features and metal foam enhances heat transfer. Reprinted from [323] with permission from Elsevier. (e) Electrically induced deformation resulting from the spatial distribution of three dielectric elastomers, optimised using phase-field driven MMTO algorithm. Reprinted from [128] with permission from Elsevier. (f) A flytrap soft active shell structure consists of elastic material and ferromagnetic soft material. The extended-LS method was utilised to achieve target response to magnetic field. Reprinted from [119] with permission from Elsevier. (g) Elastic metamaterial unit cell consisting of an array of resonators connected by thin bars. The particle swarm algorithm was applied to optimise suspension thickness and material for attenuated structural vibration. Prototype fabricated using multi-material 3D inkjet printing. Reprinted from [324] with permission from Elsevier.

Research challenges that cause deviations in the performance of manufactured products from optimised computational outcomes have been identified.

Key insights drawn from this review are summarised as follows:

- The most prominent MMTO method is SIMP, in which the voxel representation offers high adaptability for complex designs involving continuous material composition or multi-scale structures. Studies in boundary-controlled LS methods addressed interface modelling and stress constraints but overlooked other aspects like anisotropy, manufacturability, and robustness.
- ML-based inverse design strategies, whether in their standalone usage or hybridisation with numerical methods, show promise in designing multi-material lattice structures with functional grading. They enable faster design iterations by using surrogate models to accelerate evaluation or by bypassing iterative optimisation workflows altogether.
- AM processes vary in their maturity level for multi-material applications. PBF and DED are well-studied for metals while material jetting has been extensively investigated for polymers. All three processes offer intra-layer multi-material capability.
- To reduce discrepancy from virtual design to physical products, it is essential to move beyond typical assumptions made, such as perfectly-bonded interfaces, isotropic material properties, linear elastic loading, and deterministic optimisation (without uncertainty). Moreover, considerations regarding manufacturability must be addressed early in the design stage.

To advance DfMMAM principles for future engineering applications, the following research directions are suggested:

- Optimisation frameworks should accommodate diverse objectives and constraints to meet broader functional demands. The potential of multi-material in multi-objective optimisation is under-explored, with only a few studies limited to thermomechanical applications. Multi-physics coupling should be integrated. Failure-constrained design (e.g. stress, fracture, fatigue) is essential for ensuring the practical applicability of multi-material structures.
- Mechanical testing standards specific to MMAM need to be formulated to standardise interfacial property characterisation. Material and process factors require further investigation to explain failure mechanism involved in multi-material structures. Experimental findings on interfacial properties (e.g. hardness,

bonding strength) need to be integrated into the optimisation frameworks for accurate modelling. Interface control strategies require further development such that incompatible material pairs or unfavoured interfacial loading conditions can be effectively regulated.

- Additively manufactured components must be designed considering process limitations at the conceptual design stage. Process-induced anisotropy, potentially mitigated but not fully eliminated through heat treatments, remains under-researched. While there are extensive techniques on LSC, other MMAM process-specific constraints and robustness in printing receive less attention.
- Build confidence in computational results via experimental verification, fostering collaborative research between domain expertise. Encourage MMAM adoption beyond structural applications. Streamline the digitalisation workflow by advancing MMAM-specific file formats and CAD/CAM software.
- A trade-off between computational efficiency and solution optimality needs to be realised for large-scale multi-material applications. ML models demonstrate significant potential in surrogate modelling and inverse design for metamaterials, where similar strategies are suggested for DfMMAM. Parallel computing and GPU acceleration show promise in the single-material TO workflow but have not yet been explored within the multi-material context.

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Author contributions

CRedit: **Xiaochen Yu:** Conceptualization, Data curation, Formal analysis, Investigation, Software, Validation, Visualization, Writing – original draft; **Jacklyn Griffiths:** Conceptualization, Formal analysis, Investigation, Validation, Visualization, Writing – original draft; **Guha Manogharan:** Conceptualization, Funding acquisition, Resources, Supervision, Writing – review & editing; **Ajit Panesar:** Conceptualization, Funding acquisition, Project administration, Resources, Supervision, Writing – review & editing.

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Data availability

The data supporting the findings in Section 2.1.7 Benchmarking representative MMTO methods were derived from publicly available codes associated with the publications at <https://doi.org/10.1007/s00158-013-0999-1> (AAP) and <https://doi.org/10.3390/app14020657> (MM-SIMP).

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