Design of Multiphysical Coupled Metamaterials: A Review

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Abstract

Metamaterials are engineered structures with properties not found in natural materials, derived from their unique microstructural designs. Initially centered on electromagnetic applications, the field has expanded to include mechanical, thermal, and acoustic properties, enabling innovations like cloaking and programmable responses for diverse applications in optics, aerospace, and energy management. Recently, research has focused on multiphysical coupled metamaterials to address real-world needs for multifunctional materials capable of responding to multiple stimuli. Strategies such as AI-driven methods have advanced the field, allowing for adaptable, multifunctional structures. This review categorizes current research and explores future prospects for multiphysical metamaterials.

1 Introduction

Metamaterials are artificially engineered structures that possess properties not typically found in natural materials. Unlike conventional materials whose behavior is determined by their chemical composition, the unique characteristics of metamaterials arise from the specific design of their microstructures, known as meta-atoms[22]. The concept of metamaterials dates back to the theoretical work of Veselago in 1968, who predicted the possibility of materials with simultaneously negative permittivity and permeability[2]. This idea laid the foundation for subsequent developments, with the first practical demonstrations appearing decades later.

Metamaterials have since expanded beyond their initial focus on electromagnetic properties. They now encompass a broad range of applications, including mechanical, acoustic, thermal, and diffusion properties[25]. These materials exhibit extraordinary properties such as negative refractive index, cloaking, and programmable mechanical responses. For example, mechanical metamaterials can achieve ultra-lightweight structures with high stiffness or unique responses such as negative Poisson's ratio and negative stiffness.

Applications of metamaterials are diverse and transformative. In the optical domain, they enable the development of superlenses that surpass diffraction limits, invisibility cloaks, and devices for advanced wave manipulation. Mechanical metamaterials are applied in areas requiring adaptive structural responses, such as aerospace, robotics, and protective gear[4]. Thermal metamaterials are utilized for innovative heat management solutions, including cloaking and energy concentration, which find applications in electronics and sustainable building materials. This convergence of structural engineering, materials science, and physics has made metamaterials a rich area of interdisciplinary research with significant implications for future technological advancements.

Metamaterials can be categorized into various types based on their functional domains, such as elastic, thermal, electromagnetic, and acoustic metamaterials. Each of these classes exhibits unique properties that extend the capabilities of traditional materials. However, recent advancements have driven an increasing focus on the design of metamaterials that integrate multiple physical field responses—known as multiphysical coupled metamaterials.

The motivation for this shift stems from the limitations of conventional metamaterials, which are typically designed to optimize a single property. In real-world applications, structures often need to respond to multiple stimuli or achieve multiple functional objectives simultaneously. For example, aerospace and automotive components may require materials that are both lightweight and capable of thermal regulation and mechanical robustness. To address these needs, researchers have started integrating different physical properties, such as combining mechanical and thermal responses or embedding electrical functionalities within structural designs[15].

The current state of multiphysical metamaterial research highlights a range of innovative strategies. Advancements in additive manufacturing and computational design have played a critical role in enabling complex architectures that can simultaneously exhibit mechanical, thermal, and other properties. This interdisciplinary approach is pushing the boundaries of traditional materials science and enabling novel applications across engineering, robotics, and smart infrastructure.

The trend towards multiphysical designs points to a future where metamaterials can dynamically adapt to their environment and application-specific needs, providing tailored, programmable responses that were previously unattainable in natural or conventional synthetic materials.

In this review, we systematically explore the current state of research in the design and development of multiphysical coupled metamaterials. The content is structured as follows: Section 2 categorizes current research from the perspective of the problems being addressed, dividing it into two main types of studies. The first type focuses on the design of metamaterials that inherently possess different physical properties, such as combining mechanical, thermal, or electromagnetic characteristics to create multifunctional materials. The second type covers the design of metamaterials that are responsive to different external physical fields, allowing them to adapt or change their behavior in response to stimuli like temperature, electromagnetic fields, or mechanical stress. Section 3 classifies research based on the methodologies used to address these problems. The first category discusses inverse design approaches rooted in finite element analysis and homogenization theory, which are foundational for optimizing material structures for specific properties. The second category highlights artificial intelligence (AI)-enhanced methods, particularly those integrating deep learning, which have opened up new possibilities for exploring complex design spaces and achieving rapid design iterations. Finally, Section 4 provides a summary of the current advancements and discusses potential future research directions.

2 Classification of Problems in Current Research

The development of metamaterials with the ability to manipulate multiple physical properties simultaneously has led to significant breakthroughs in various fields, but it has also presented unique challenges. The problems of interest can be divided into two categories: the design of metamaterials that inherently possess different coupled physical attributes and the development of metamaterials that respond dynamically to external physical fields. These areas represent the core challenges in advancing multiphysics applications and highlight the intersection of material science, engineering, and physics.

2.1 Design of Metamaterials with Multiphysical Properties

In recent years, the design of metamaterials with single physical properties has achieved notable success, enabling advancements in areas such as negative refraction and cloaking. However, many practical applications require materials that can simultaneously manage multiple physical phenomena, such as mechanical, thermal, and electromagnetic properties. This necessity has driven research toward developing metamaterials with multiphysical capabilities, aiming to create multifunctional devices for applications like adaptive optics, thermal management, and energy harvesting.

2.1.1 Coupling of Mechanical and Thermal Properties

Coupling mechanical and thermal properties in metamaterials allows for simultaneous control of stress distribution and heat flow. This type of integration is crucial for applications in environments that require efficient thermal management without compromising structural integrity, such as aerospace and automotive industries. Innovations include composite structures designed for customized thermal conductivity and mechanical strength, enabling better heat dissipation and structural resilience. Zhao et al. (2023)[26] developed a scalable, high-porosity wood material, insulwood, that exhibits exceptional sound absorption, thermal insulation, and mechanical strength. Created through a rapid delignification and ambient drying process, insulwood maintains structural integrity, making it suitable for sustainable building applications. Although distinct from topology optimization methods, this work highlights the practical potential of materials combining strong mechanical and thermal properties for energy-efficient construction.

Sigmund and Torquato (1996)[12] first showed that there is no mechanistic relationship between negative thermal expansion and negative Poisson's ratio. Wang et al. (2004)[20] developed a multi-phase level-set model with an objective function that includes both mechanical and thermal components, demonstrating examples with specified thermal expansion coefficients and negative Poisson's ratios. Álvarez Hostos et al. (2021)[30] utilized topology optimization to design manufacturable thermo-mechanical metadevices that effectively control displacement under thermal gradients. Wang et al. (2024)[21] used deep learning techniques to design thermal metamaterials that maintained original thermal performance while achieving enhanced mechanical properties, such as load-bearing capacity, shearing strength, and tensile resistance.

2.1.2 Coupling of Electrical and Thermal Properties

Materials that possess specified electrical and thermal conductivities have a wide range of potential applications, particularly in fields that require precise management of both electrical and thermal energy. For example, in electronic devices, materials with tailored electrical and thermal properties are essential for efficient heat dissipation and stable electrical performance, preventing overheating and improving overall device longevity. Thermal management systems in power electronics and batteries also benefit from such materials, ensuring effective temperature regulation while maintaining electrical conductivity. Additionally, smart textiles and wearable electronics use these materials to provide integrated thermal control and energy transmission, enhancing comfort and functionality in flexible, user-friendly formats. In energy harvesting and thermoelectric devices, materials that can simultaneously optimize electrical and thermal conductivities play a crucial role in converting temperature gradients into electrical energy with high efficiency.

The design of materials that have both specified electrical and thermal conductivities is relatively more straightforward compared to other multiphysical combinations due to the mathematical similarities between the equations governing electrical and thermal transport. Both processes are described by similar differential equations, with electrical conductivity governed by Ohm's law and thermal conductivity by Fourier's law. This analogy allows for the adaptation of design methods developed for one type of transport to the other, facilitating the creation of dual-function materials. Researchers can leverage this similarity to design metamaterials that balance electrical and thermal behavior, maintaining tailored conductivities across different scales and applications.

Torquato et al. (2002)[17] explored optimizing three-dimensional, two-phase composites to enhance the simultaneous transport of heat and electricity, introducing topology optimization methods and identifying bicontinuous structures as optimal for combined conductivity. Zhu et al. (2023)[29] advanced this by designing general transformation multiphysics metamaterials that manipulate multiple physical fields like heat and electric current. Unlike Torquato et al., Zhu et al. employed a "discretion-and-assembly" strategy to create complex, shape-flexible structures with diverse functionalities, moving beyond static property optimization to adaptable, multifunctional designs.

2.2 Design of Metamaterials Responsive to Physical Fields

The mechanical metamaterials in which on-demand effective property modulation can be realized even after manufacturing are the ones with active property modulation. This can be achieved by using active materials in the unit cells and activating them through external stimuli like magnetic or electric fields. Recent studies in this field include the coupling of stimuli-responsive materials with the design of unit cell based microstructural configuration of mechanical metamaterials. Under the external stimulus, these metamaterials can show unconventional characteristics and thus can be put to use as per different application-specific requirements based on live operational demands. The external stimuli can be pressure action, heat, light, magnetic field, electric current, and chemicals. Further, shape memory alloys can be used in metamaterials for achieving active behavior including shape morphing. Note that such active property modulation often entails the multi-physical behaviour of mechanical metamaterials including the mechanics of deformation under mechanical load and non-mechanical stimuli. This multi-physical behavior at the elementary beam-level and the micro-scale unit cell level can thus manifest unprecedented active properties at the macro-scale metamaterial-level through a bi-level design paradigm. In the following subsections, we discuss the recent progress in the multi-physical behavior of active metamaterials under different external stimuli.

2.2.1 Responsive to temperature

Materials with varying mechanical properties at different temperatures have a range of practical applications. One prominent application is in adaptive structures, such as components in aerospace and automotive industries, where materials need to maintain mechanical integrity under fluctuating temperatures. These materials are used to create thermal actuators in robotics, which can respond to temperature changes to produce controlled movements or adjust stiffness. The ability to design materials that respond to temperature variations is made possible by combining materials with different thermal expansion coefficients or distinct glass transition temperatures. This strategy enables the creation of composites or metamaterials that exhibit tailored responses to heat.

Yang et al. (2019)[23] developed lightweight 4D-printed active lattices with significant temperature-dependent stiffness variation and reconfigurable mechanical properties. Tao et al. (2020)[16] developed 4D-printed SMP-based origami metamaterials with tunable mechanical properties, enabling temperature-controlled adjustments in stress-strain curves and compression twist behavior for adaptive structural applications. Li et al. (2023)[8] developed a multimaterial topology optimization framework to design 3D-printed metamaterials capable of specified force-displacement curves at different temperatures, leveraging polymers with distinct glass transition temperatures for adaptive mechanical responses.

2.2.2 Responsive to electric field

Electrically actuated metamaterials work on the principle of change in mechanical behavior induced by electric field. Thus the multiphysical aspect of these metamaterials gets involved since electrical, thermal and mechanical forces are coupled to give unconventional deformation characteristics. They can be broadly of two types as follows. In the first category, mechanical deformation occurs by the use of thermal energy produced by current in conductors. Thus these are essentially thermally actuated metamaterials where the temperature is generated through electrical fields. The other category gets triggered by external electrical actuation caused by chemical or physical reactions. These include electroactive polymers, electrochemically stimulated materials and ionic polymer-metal composite materials.

Levine et al. (2021)[7] provided an in-depth review of electroprogrammable stiffness materials, categorizing them by mechanisms and evaluating their applications, while highlighting the balance between response time, power consumption, and stiffness modulation. Singh et al. (2021)[14] developed a hybrid lattice microstructure incorporating piezoelectric materials for voltage-dependent modulation of elastic properties, introducing programmable state transitions in Young's moduli via a novel multiphysics analytical framework.

2.2.3 Responsive to magnetic field

Magnetic field-responsive metamaterials function through mechanical behavior modulated by applied magnetic fields, coupling magnetic forces with mechanical responses to achieve unique deformation patterns. These materials are essential for applications requiring remote, untethered control of movement or shape change, such as soft robotics, biomedical devices, and adaptive structural systems.

Zhao and Zhang (2022)[27] developed a topology optimization framework that simultaneously optimizes the topology, remnant magnetization distribution, and applied magnetic fields for hard-magnetic soft materials. This approach supports the creation of programmable, shape-morphing structures and magnetic actuators that achieve complex deformation modes under large deformations. The design framework significantly expands the design space, enabling more effective actuation and multifunctional capabilities.

Wang et al. (2023)[18] extended the inverse design of magneto-active metasurfaces by introducing a multi-physics topology optimization framework that optimizes geometry, magnetization distribution, and magnetic field parameters. Their method allows for precise 3D shape morphing, supporting applications such as bio-inspired robots with various motion types. The validation through experiments highlighted the feasibility of achieving programmable deformations, showcasing how magnetic-responsive metamaterials can be fine-tuned for high-precision actuation.

3 Classification by Methods Used

From the above introduction to specific works, it can be seen that our research methods can be mainly divided into two categories. The first category is inverse design methods based on finite element analysis and homogenization theory, which focus on systematically optimizing material structures to achieve desired properties. The second category involves methods that integrate artificial intelligence, such as deep learning, to enhance the design process. These AI-driven approaches allow for the exploration of large design spaces and facilitate the rapid generation of innovative solutions that traditional optimization methods may not easily achieve. Next, we will provide a detailed introduction to each category.

3.1 Inverse Design Based on Homogenization Theory

Homogenization theory has been a foundational tool in material science, particularly in the design of metamaterials that exhibit tailored macroscopic properties derived from complex microstructures. This theory originated as a means to understand and model the effective behavior of composite materials, where the material's properties at a macro scale are influenced by the arrangement and characteristics of its microscale constituents. Over time, homogenization theory has evolved, incorporating advanced mathematical models and computational tools to address more complex design challenges, including those involving multiple interacting physical fields.

The effectiveness of inverse design based on homogenization theory is evident in its capacity to create metamaterials with highly customizable properties[13]. By leveraging numerical simulations and optimization algorithms, researchers can design microstructures that meet specific criteria, such as mechanical stiffness, thermal conductivity, and even anisotropic behavior. This method has enabled significant advancements in engineering applications, including lightweight structural components, advanced thermal insulators, and energy-absorbing materials. The use of homogenization theory allows for the precise calculation of effective properties and aids in bridging the gap between theoretical material behavior and practical implementation.

Despite its strengths, there are notable limitations when applying inverse design methods based on homogenization theory to multiphysical coupling problems. One significant challenge is the inherent complexity of modeling interactions between different physical fields, such as mechanical and thermal properties, which often require distinct and sometimes conflicting microstructural designs. While homogenization can approximate effective properties for each field individually, integrating these into a coherent design that functions optimally under simultaneous multiphysics conditions remains difficult. Additionally, the computational cost of simulating these coupled interactions can be prohibitive, especially as the complexity of the material's microstructure increases. This method also struggles with non-linear behavior and can face limitations when predicting responses under dynamic or highly variable external conditions. As a result, while inverse design using homogenization theory has proven powerful, its application to multiphysical scenarios often requires supplementary methods or hybrid approaches to achieve satisfactory results.

3.2 Use of Deep Learning Techniques

To address the limitations of inverse design based on homogenization theory, particularly in handling complex multiphysical interactions, researchers have introduced artificial intelligence (AI) methods. The rapid advancement of AI, and deep learning (DL) in particular, has offered new avenues for overcoming these challenges. Deep learning, which is a subset of machine learning, has seen significant progress over the past decade, achieving remarkable success in various fields, most notably in image processing. Its ability to analyze and generate high-dimensional data has revolutionized fields such as computer vision, natural language processing, and more.

The success of deep learning in image processing is particularly relevant to its application in topology optimization. The mathematical nature of design variables in topology optimization, represented as matrices of material distributions, closely mirrors that of images, which are also expressed as pixel matrices. This similarity has facilitated the use of deep learning frameworks for topology optimization, where neural networks can learn complex mappings between input parameters and optimal design outputs. Deep learning models can explore vast design spaces, predict optimal material distributions, and even discover novel topologies that traditional methods might overlook. Moreover, DL techniques can handle the non-linearities and complex interactions inherent in multiphysical problems, providing an adaptable framework for real-time design optimization.

Commonly used deep learning frameworks in topology optimization include Generative Adversarial Networks (GANs), Variational Autoencoders (VAEs)[3], Convolutional Neural Networks (CNNs), and Reinforcement Learning (RL). Variants and specialized models, such as Conditional GANs (cGANs), Deep Convolutional GANs (DCGANs), Bayesian Neural Networks, U-Net architectures, Graph Neural Networks (GNNs), and Physics-Informed Neural Networks (PINNs), have also been employed[6][1]. These frameworks are tailored to solve specific problems, enabling the generation of complex designs, learning of latent variable representations, and prediction of multi-field interactions in topology optimization.

In traditional topology optimization methods, whenever boundary conditions or applied loads change, it is necessary to start complex finite element calculations from scratch to obtain the final optimized structure. In contrast, deep learning methods learn the mapping from certain inputs to the final optimized structure. Although the training process relies on using traditional topology optimization methods to generate the dataset, which still involves significant computation, once the model is trained, it becomes easy to obtain new optimized structures based on new boundary conditions, and real-time design can even be achieved.

We have observed that the "certain inputs" in the mapping from inputs to the final optimized structure have evolved in the literature. Rawat and Shen (2019)[11] utilized a conditional Wasserstein GAN to solve the simplest topology optimization problem, using volume fraction, SIMP penalization, and filter radius as parameters while keeping boundary conditions fixed. Yu et al. (2019)[24] developed a two-part deep learning method using volume fraction and boundary conditions as parameters, combining a CNN for low-resolution prediction and a cGAN for upscaling to high resolution in topology optimization. Nie et al. (2020)[9], motivated by the limitations of representing input displacement and load boundary conditions as sparse matrices—which hinder networks from capturing spatial variations and physical phenomena within the material domain—introduced TopologyGAN, a conditional GAN-based framework. This method incorporated detailed physical field data, such as von Mises stress and strain energy density, as input to improve the accuracy of mappings from boundary conditions to optimized topologies. Additionally, the use of a U-SE-ResNet hybrid generator architecture enhanced model performance, resulting in significant error reductions and effective handling of unseen boundary conditions. Kazemi et al. (2022)[5] investigated the use of single-physics and multiphysics data in the training of their GAN for topology optimization of thermoelastic structures. Inherently, coupled multiphysics training data are more computationally demanding to create. Thus, they analyzed the extent to which single-physics data, combined with a limited number of multiphysics samples, could be used to train a GAN for multiphysics design optimization. To this end, they reduce the front end computational demand of data generation for this approach, with minimal sacrifice in quality of generated designs. Parrott et al. (2023)[10] utilized style transfer to migrate the design style or features of a single-physics field to another design, enabling the rapid generation of multiphysics optimization.

Despite their advantages, deep learning methods in topology optimization are not without limitations. One major challenge is the dependency on high-quality, extensive datasets for training, which are often generated using traditional computational methods such as finite element analysis. This process can be computationally expensive and time-consuming, limiting the scalability of deep learning approaches. Additionally, deep learning models can act as "black boxes," making it difficult to interpret how design decisions are made and to ensure that the generated solutions are physically valid or practical for manufacturing. Another issue is the generalizability of these models; while they may perform well under conditions similar to those in the training set, their performance may degrade when faced with entirely new scenarios or more complex multiphysics interactions. Addressing these issues requires integrating domain knowledge, physics-based constraints, and hybrid approaches that combine traditional optimization with machine learning to create more transparent, reliable, and versatile design tools.

4 Conclusion and Future Outlook

Metamaterials, particularly multiphysical coupled metamaterials, hold immense potential for future research and practical applications. This review has outlined current research categorized by problem focus—designing materials with different intrinsic properties and creating materials that respond to multiple external fields—and by methodology, including inverse design approaches and AI-enhanced methods. The vast range of physical properties and their combinations theoretically opens up countless research possibilities. However, the significance and impact of these studies must be evaluated carefully, with an emphasis on an application-driven approach to selecting meaningful research problems. This ensures that research outcomes are not only novel but also relevant and beneficial in real-world scenarios.

One effective strategy for broadening research scope is adapting existing methodologies to new domains. For instance, solutions developed for thermal responses could be applied to electromagnetic contexts or expanded to scenarios involving both thermal and electromagnetic responses. Similarly, advances in mechanical cloaking[19] and thermal cloaking[28] could inspire research into more complex systems that integrate mechanical, thermal, and electromagnetic cloaking. These efforts rely on leveraging current frameworks while exploring their adaptability to more intricate physical interactions.

While starting with established methods is common, research must move beyond superficial replication. Researchers need a thorough understanding of the underlying physics involved in these transitions to foster meaningful modifications and innovations. This deep knowledge can push the boundaries of current work, leading to genuinely novel insights.

Deep learning continues to be a powerful tool in metamaterial design, offering potential that is yet to be fully exploited. There are opportunities to enhance the scalability and versatility of deep learning-based approaches, making them better suited for complex, multiphysical scenarios. However, achieving groundbreaking progress will require sustained, rigorous work that encourages new ideas and inspiration. Over time, consistent and insightful research will lead to fundamental advancements, opening new frontiers in the study and practical applications of multiphysical coupled metamaterials.

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