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AI-Enabled Design and Additive Manufacturing of Mechanical Materials: Methods and Future Directions

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Abstract

This review provides a comprehensive overview of recent advancements in the development of mechanical metamaterials through the synergistic integration of artificial intelligence (AI) and additive manufacturing (AM). By combining computational design strategies with high-precision fabrication techniques, researchers can rapidly identify optimized microstructures and translate them into functional prototypes. This approach accelerates the exploration of multifunctional and adaptive metamaterials, enabling properties that are difficult to achieve with conventional materials. This paper highlights key methodologies for AI-assisted design and AM-based fabrication, examines their capabilities and limitations, and outlines workflows that bridge theoretical modeling and practical implementation. Emerging trends, including self-adaptive metamaterials and application-specific architectures, are discussed to provide guidance for future research. Overall, this review emphasizes how AI and AM collectively transform the landscape of mechanical metamaterial design, offering pathways toward faster innovation, enhanced performance, and real-world applicability.

Keywords

mechanical metamaterials, artificial intelligence, additive manufacturing, topology optimization

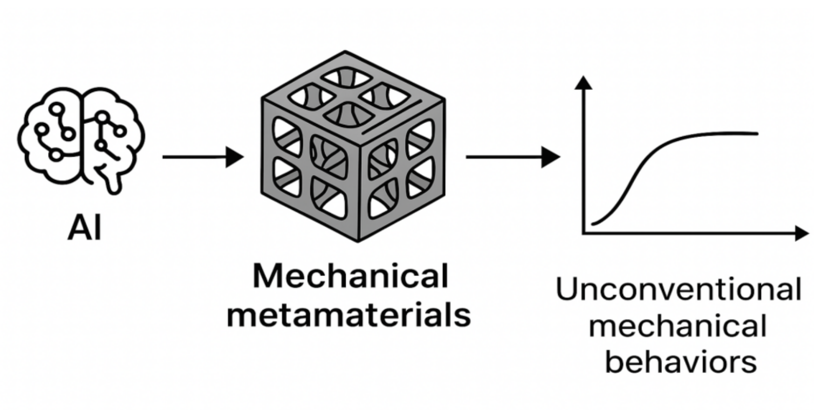
1. Introduction

Mechanical metamaterials are artificially engineered structures with architected micro- and nanoscale geometries that endow them with unconventional mechanical behaviors unattainable in natural materials (Bertoldi et al., 2017). Unlike conventional materials, whose properties are primarily determined by their intrinsic chemical composition, the remarkable performance of mechanical metamaterials arises predominantly from their designed structural topology, hierarchical arrangement, and multiscale geometrical features. In recent years, mechanical metamaterials have emerged as research and application hotspots owing to their superior mechanical properties and functionalities, with transformative applications across diverse fields, including aerospace engineering and civil infrastructure (Jiao et al., 2023).

With the rapid development of artificial intelligence and additive manufacturing technologies, the paradigm of metamaterial design and fabrication is undergoing a profound transformation. AI-driven computational models, such as deep learning, reinforcement learning, and generative design algorithms, enable accelerated inverse design, topology optimization, and the computational discovery of novel architectures. Complementing these advances, additive manufacturing technologies-including high-resolution 3D printing, multimaterial printing, and two-photon lithography-provide the precision, geometric freedom, and scalability necessary to physically realize these intricate designs. As shown in Figure 1, the synergy between artificial intelligence and additive manufacturing not only bridges the gap between theoretical design and practical implementation but also accelerates the development of next-generation mechanical metamaterials with tailored, multifunctional, and adaptive properties.

This paper reviews the recent advances in AI-enabled design and additive manufacturing of mechanical metamaterials, discusses their synergistic integration, analyzes current challenges, and outlines future research directions.

Figure 1: Schematic illustration of the AI–AM–mechanical metamaterial pipeline.



2. Body of Paper

2.1 AI-Enabled Design of Mechanical Materials

The design of mechanical metamaterials is inherently complex, as their extraordinary properties emerge not from their chemical composition but from carefully engineered geometrical arrangements across multiple scales. Conventional trial-and-error or purely physics-based optimization approaches often face challenges of high computational cost, limited design space exploration, and lack adaptability to evolving functional requirements. Artificial intelligence (AI) provides a paradigm shift by enabling data-driven, predictive, and generative approaches that significantly accelerate and enrich the design workflow.

2.1.1 Machine Learning for Property Prediction

Machine learning (ML) algorithms have been increasingly applied to establish predictive models that map structural descriptors of metamaterials to their effective mechanical properties. Supervised learning techniques-such as regression-based models, random forests, and support vector machines-enable fast evaluation of elastic moduli, Poisson's ratios, and energy absorption capacities on the basis of training datasets generated from finite element simulations or experimental measurements (Zhang and Zhao, 2024). This predictive capability allows researchers to screen vast design spaces efficiently, thereby reducing the reliance on exhaustive simulations. Moreover, transfer learning has emerged as a powerful tool for adapting models trained on one class of metamaterials to related but structurally distinct classes, further enhancing the efficiency of predictive modeling.

2.1.2 Deep Learning and Inverse Design

Deep learning (DL) architectures, particularly convolutional neural networks (CNNs) and graph neural networks (GNNs), have been employed for the inverse design of metamaterials. Unlike forward prediction models, inverse design focuses on determining the optimal microstructure that yields a target set of properties. Variational autoencoders (VAEs) and generative adversarial networks (GANs) provide the capacity to automatically generate novel microstructures beyond human intuition, enabling the discovery of unconventional yet functional architectures (Zhang and Zhao, 2024). Reinforcement learning (RL) further extends this paradigm by framing the design process as a sequential decision-making problem, in which an AI agent iteratively improves the geometry on the basis of feedback from simulated or experimental performance metrics.

2.1.3 Multiobjective and Topology Optimization

Mechanical metamaterial design often requires balancing multiple objectives, such as maximizing stiffness while minimizing weight or optimizing both strength and energy absorption. Traditional topology optimization methods, while powerful, are computationally intensive for complex geometries. AI-driven surrogate models and hybrid approaches combine the rigor of physics-based methods with the efficiency of machine learning to achieve real-time multiobjective optimization. These methods significantly expand the design space and facilitate the creation of hierarchical and multifunctional architectures that would be infeasible to obtain through conventional optimization alone.

2.1.4 Integration of AI with Physics-Informed Models

While purely data-driven methods offer speed and adaptability, they may lack interpretability and generalizability outside the training domain. Recent advances emphasize the integration of AI with physics-informed neural networks (PINNs) and reduced-order modeling techniques, which embed governing physical laws into the learning process. This hybrid paradigm ensures that AI-generated designs remain physically feasible, robust under varying boundary conditions, and better aligned with practical manufacturing constraints.

2.2 Additive Manufacturing Techniques for Metamaterials

Additive manufacturing (AM) has emerged as a critical enabling technology for the physical realization of mechanical metamaterials, offering unprecedented geometric freedom, multimaterial integration, and high spatial resolution. Unlike traditional subtractive manufacturing methods, AM builds structures layer by layer, allowing the fabrication of intricate lattice networks, hierarchical architectures, and functional gradients that are essential for achieving the desired mechanical properties. This section reviews key AM technologies and their applications in metamaterial fabrication.

2.2.1 High-resolution 3D printing

High-resolution 3D printing techniques, including stereolithography (SLA), digital light processing (DLP), and two-photon polymerization (2PP) (Hussain, 2024), enable the fabrication of micro- and nanoscale metamaterial features with submicron precision. SLA and DLP utilize photopolymerization of liquid resins to create complex lattices rapidly, whereas 2PP offers unparalleled resolution and is capable of producing nanostructured architectures that are otherwise unattainable with conventional methods. These technologies are particularly suitable for producing lightweight, high-strength metamaterials with controlled deformation mechanisms and tunable mechanical responses.

2.2.2 Multimaterial and Functionally Graded Printing

The integration of multiple materials within a single building allows the creation of metamaterials with spatially varying mechanical, thermal, or electrical properties. Multiple-material AM techniques, such as PolyJet printing and inkjet-based material jetting, facilitate the combination of soft and stiff phases, enabling the realization of functionally graded structures that mimic natural hierarchical systems. This capability is crucial for designing metamaterials that exhibit programmable stiffness, shape-morphing behavior, or energy absorption tailored to specific applications.

2.2.3 Metal and Ceramic Additive Manufacturing

For applications demanding high strength, wear resistance, or thermal stability, metal and ceramic AM processes, such as selective laser melting (SLM), electron beam melting (EBM), and binder jetting (Bandyopadhyay et al., 2023), are increasingly employed. These methods allow the fabrication of load-bearing metamaterials with complex lattices and internal voids that are suitable for aerospace, automotive, and civil engineering applications. Postprocessing techniques, including heat treatment and hot isostatic pressing, further enhance the mechanical performance and surface quality, ensuring the functional reliability of the printed metamaterials.

2.2.4 Process–Property Integration and Design for Manufacturability

A critical aspect of AM for metamaterials is the tight coupling between process parameters and the resulting material properties. Factors such as layer thickness, laser power, scan speed, and material viscosity directly influence feature resolution, internal porosity, and mechanical performance. Design-for-manufacturability (DFM) strategies are therefore essential, enabling designers to anticipate and mitigate fabrication defects while maintaining fidelity to the intended microarchitecture. Coupling AI-enabled design with AM process optimization facilitates the production of metamaterials that efficiently meet both structural and functional requirements.

2.2.5 Emerging Trends in Additive Manufacturing for Metamaterials

Recent advancements in AM are pushing the boundaries of metamaterial fabrication toward adaptive, multifunctional, and self-healing systems. Innovations such as in situ monitoring, real-time feedback control, and hybrid additive-subtractive processes enhance precision, reproducibility, and scalability. Furthermore, combining AM with postprocessing techniques such as chemical infiltration, surface coating, or material doping expands the range of achievable mechanical and functional properties. These developments pave the way for application-specific metamaterials that can respond dynamically to environmental stimuli or load conditions.

2.3 Integration of AI and Additive Manufacturing for Mechanical Metamaterials

The convergence of artificial intelligence and additive manufacturing represents a transformative paradigm in mechanical metamaterial research. By linking computational design, predictive modeling, and high-fidelity fabrication, this integrated approach enables the rapid realization of complex, multifunctional, and application-specific architectures that would be infeasible with traditional methods alone.

2.3.1 Digital Twin Frameworks

Digital twin technology enables real-time simulation of manufacturing processes in a virtual environment. By integrating artificial intelligence (AI), it can predict process parameters, monitor the manufacturing process, and use real-time feedback data from additive manufacturing to update the model and correct any deviations, thus improving the efficiency of design and manufacturing collaboration and achieving closed-loop control for enhanced process stability. For example, Liu et al. (2024) proposed a closed-loop digital twin control framework for laser powder bed fusion (L-PBF) processes based on deep neural networks (Liu et al., 2024).

In the digital manufacturing ecosystem, AI and additive manufacturing (AM) technologies play crucial roles through integration with digital twin (DT) technology.

2.3.2 Closed-Loop AI–AM Design Workflow

A closed-loop AI–AM workflow integrates machine learning models with in situ process monitoring and postfabrication characterization. AI predicts the impact of geometric variations and process parameters on mechanical performance, whereas AM systems provide immediate feedback on printing fidelity and structural integrity. Reinforcement learning frameworks can exploit this feedback to iteratively refine microstructures, optimizing for multiobjective criteria such as the stiffness–to–weight ratio, energy absorption, and fatigue resistance. Such workflows substantially reduce design cycles and enable the production of robust, application-specific metamaterials.

2.3.3 Multiscale Optimization and Hierarchical Design

The integration of AI and AM facilitates multiscale optimization, allowing metamaterials to be engineered across the nanoscale, microscale, and macroscale scales simultaneously. Hierarchical architectures, with tailored unit cells, gradient structures, and functional interfaces, can be computationally generated via generative models and realized via high-precision AM techniques. This approach enables the concurrent tuning of global mechanical behavior and local functional responses, resulting in metamaterials with unprecedented combinations of stiffness, strength, energy absorption, and adaptability.

2.3.4 AI-Guided Material Selection and Process Parameterization

In addition to structural design, AI can assist in selecting suitable materials and optimizing AM process parameters to achieve the desired metamaterial performance. By leveraging predictive models trained on experimental and simulation datasets, AI can recommend material compositions, printing strategies, and postprocessing steps that maximize mechanical efficiency while minimizing defects. This synergistic approach ensures that both the architecture and the fabrication process are cooptimized, reducing manufacturing costs and improving the reliability of the final product.

2.3.5 Challenges and Opportunities in AI–AM Integration

Despite its potential, the full integration of AI and AM for mechanical metamaterials faces several challenges. These include limited high-quality datasets for training AI models, computational costs associated with multiobjective optimization, and scaling constraints in AM for large or complex structures. Addressing these issues requires advances in physics-informed machine learning, high-throughput experimental characterization, and hybrid fabrication techniques. Nonetheless, the continued convergence of AI and AM holds enormous promise for enabling next-generation metamaterials with tailored, adaptive, and multifunctional properties suitable for aerospace, biomedical, civil, and energy applications.

2.4 Future Directions and Perspectives

The intersection of artificial intelligence and additive manufacturing has unlocked unprecedented opportunities in the design and fabrication of mechanical metamaterials. Looking forward, several research directions and emerging trends are expected to shape the field over the next decade.

2.4.1 Self-Adaptive and Stimuli-Responsive Materials

Future mechanical metamaterials are expected to exhibit self-adaptive or stimuli-responsive behavior, enabling real-time adjustment of mechanical properties in response to external stimuli such as load, temperature, or magnetic fields. AI-guided design can predict optimal microstructural configurations for adaptive functionality, whereas advanced AM techniques allow the fabrication of responsive unit cells with integrated actuation mechanisms. These metamaterials hold promise for applications in soft robotics, wearable devices, and impact mitigation systems.

2.4.2 Multifunctional and Multiphysics Integration

The next generation of metamaterials will increasingly integrate multiple functionalities, such as combined mechanical, thermal, acoustic, and electrical properties. AI-driven multiphysics modeling and optimization can guide the design of metamaterials that simultaneously satisfy diverse performance criteria, whereas AM enables the precise placement of heterogeneous materials and gradients at multiple scales. These multifunctional metamaterials could revolutionize aerospace components, energy harvesters, and biomedical implants.

2.4.3 High-Throughput Autonomous Design-to-Fabrication Platforms

To accelerate innovation, future workflows are likely to adopt high-throughput and autonomous platforms that integrate AI, AM, and real-time characterization. Automated design–fabrication–testing loops can rapidly explore vast design spaces, identify optimal architectures, and validate performance with minimal human intervention. Such platforms will dramatically reduce development timelines and enable large-scale deployment of metamaterials in industrial applications.

2.4.4 Data-Driven Materials Discovery and Sustainability

The combination of AI and AM offers transformative opportunities for data-driven mechanical material discovery, enabling the design of novel material compositions and microarchitectures guided by performance-driven objectives. AI-based generative models, surrogate predictors, and active learning platforms facilitate the rapid exploration of both structural and compositional design spaces to identify candidates optimized for mechanical, thermal, and multifunctional performance. Alongside this capability, sustainability considerations-such as recyclability, energy-efficient fabrication strategies, and lifecycle CO_2 emissions-are becoming integral to metamaterial development workflows. Recent work has demonstrated how machine learning models trained on experimental process data coupled with process parameter optimization can accurately forecast and minimize CO_2 emissions during AM operations, particularly through fine-tuning of the infill density, layer thickness, and temperature settings (Hauck et al., 2025). By integrating these sustainability-aware AI tools with AM fabrication, researchers can cooptimize the design, performance, and environmental impact of next-generation mechanical metamaterials

3. Conclusion

3.1 Research Summary

This review has examined the synergistic integration of artificial intelligence (AI) and additive manufacturing (AM) in the field of mechanical metamaterials. AI facilitates predictive modeling, inverse design, and multiobjective optimization, thereby enabling the exploration of broader design spaces; AM provides reliable technological support for the precise fabrication of complex micro- and nanoarchitectures. Their integration establishes a closed-loop design–fabrication paradigm that drives the rapid development of next-generation metamaterials with customizable, multifunctional, and adaptive properties. The novelty of this study lies in highlighting the potential of AI–AM integration and its profound impact on the future landscape of metamaterial research.

3.2 Limitations and Challenges

Despite the significant progress achieved, several limitations remain:

AI algorithms require improvements in interpretability and generalization across tasks;

High-resolution AM still faces challenges in terms of material compatibility, manufacturing efficiency, and cost control;

The design–fabrication–validation loop has not yet been fully established, and feedback mechanisms require further development.

3.3 Future Outlook

Future research may be further advanced in the following directions:

Algorithm Advancement: Development of explainable and robust AI models capable of handling multiphysics coupling problems;

Manufacturing breakthroughs: advancements in multimaterial and hybrid AM technologies to increase fabrication precision and functional diversity;

Intelligent **closed-loop systems**: Establishment of real-time, data-driven design–fabrication–testing platforms with feedback optimization;

Application **expansion**: Scaling up the practical deployment of metamaterials across the aerospace, civil engineering, biomedical, and energy sectors.

Through continuous interdisciplinary integration and technological innovation, the deep synergy between AI and AM is expected to accelerate the transition of mechanical metamaterials from laboratory research to practical engineering applications, ultimately demonstrating their value in a wide range of industrial and societal contexts.

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Conflicts of Interest

The authors declare no conflict of interest.

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