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Artificial intelligence-driven material development for additive manufacturing: A critical review

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Abstract

Additive manufacturing (AM) has revolutionized material fabrication by enabling the production of complex structures with enhanced design flexibility and material efficiency. However, the development of AM-specific materials remains a critical challenge due to the unique process characteristics of AM. Recent advancements in artificial intelligence (AI), for example, machine learning and deep learning, have emerged as powerful tools in accelerating material discovery, optimizing process parameters, and improving material performance for AM. This review provides a comprehensive overview of AI-driven material development for AM, focusing on metals, polymers, and bioinks/biomaterial inks. The discussion encompasses AI techniques applied to material development, including predictive modeling, generative algorithms, and intelligent optimization methods. Data collection and pre-processing methodologies for AI applications in AM are discussed. In addition, the applications of AI in material development in AM are also reviewed. Finally, the review highlights emerging trends, such as AI-driven high-throughput material screening, integration of AI with multiscale high-fidelity simulations, the use of digital twins for real-time process control, and active learning strategies for optimizing material compositions. By summarizing recent advancements and outlining future directions, this review provides insights into the evolving intersection of AI and AM, paving the way for more intelligent and efficient material development in the next generation of manufacturing.

Keywords: Artificial intelligence; Additive manufacturing; Machine learning; Material design; Performance optimization; Bioprinting

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1. Introduction

Additive manufacturing (AM) has revolutionized modern manufacturing by enabling the layer-by-layer fabrication of complex structures with high precision and design flexibility.[1] This approach minimizes or even eliminates the need for extensive machining, thereby significantly improving material utilization efficiency.[2] As a general term encompassing various techniques, AM has been adopted across multiple industries, including aerospace, biomedical, and automotive sectors. Each AM technique, whether designed for metals, polymers, or bioinks/biomaterial inks, operates under distinct processing principles that influence the manufacturability and performance of fabricated components.[3,4]

Designing and optimizing materials for AM remains a challenging task, as it has traditionally relied on heuristic-driven trial-and-error methods that are both time-consuming and resource-intensive. These conventional approaches struggle to efficiently navigate the complex and non-linear relationships between processing conditions, microstructure evolution, and resulting material properties. Moreover, most existing materials were originally developed for conventional manufacturing techniques and are often not suitable for AM, leading to issues such as poor printability, defect formation, and variability in mechanical performance.[5,6] The growing need for AM-specific materials with tailored functionalities demands a paradigm shift in how materials are discovered and developed. In this context, artificial intelligence (AI) offers powerful capabilities to handle high-dimensional datasets, identify hidden patterns, and accelerate the design process by predicting material performance based on compositional and process parameters. By moving beyond empirical heuristics, AI-driven methods enable more systematic and scalable exploration of the vast design space, offering a promising alternative to traditional approaches.

In recent years, AI has demonstrated remarkable success in media applications based on image and voice big data, and it has recently expanded into diverse fields, such as medicine, education, and engineering.[7,8] Its ability to analyze vast datasets, identify complex patterns, and make predictive decisions has also positioned AI as a powerful tool in scientific and industrial applications, including materials science. In particular, AI has emerged as a transformative tool in accelerating materials development for AM. By leveraging data-driven approaches, AI enables the prediction of material properties, optimization of alloy compositions, and exploration of new material spaces with reduced experimental effort. AI-driven methods facilitate the rapid identification of processable materials with tailored properties, improving the efficiency of AM applications across metals, polymers, and bioinks/biomaterial inks. As AM continues to evolve toward more sophisticated and customized applications, AI-driven material development plays an increasingly vital role in bridging the gap between computational design and experimental realization. The increasing research interest in this field is reflected in the growing number of AI-driven AM publications over the past decade, as illustrated in Figure 1.

Given the growing importance of AI in materials discovery for AM, this review aims to provide a critical assessment of recent advancements in AI-driven material development across different AM material categories. Unlike many existing reviews that predominantly focus on *in situ* monitoring, process control, or the printability assessment of feedstock materials using AI,[9] this review specifically emphasizes AI-driven material development. We adopt a narrow definition of material development, which centers on the design and optimization of material properties or compositions, excluding applications solely related to manufacturability, defect detection, or geometry control. This focused perspective highlights the unique role of AI in accelerating the discovery and tailoring of materials for AM. The framework of the review is presented in Figure 2. The discussion covers data collection and pre-processing methods, AI-enabled material development strategies, and key applications in AM. By summarizing recent progress and highlighting existing challenges, this review seeks to offer insights into the evolving intersection of AI and AM materials development, paving the way for future innovations in this field.

2. Overview of various AM techniques and the need for material development

There are various AM techniques that enable the fabrication of complex structures. Each AM technique imposes distinct material requirements, influencing processing feasibility and final part performance. This section provides a concise description of seven key AM techniques (Figure 3), their material requirements, and challenges in material development.

2.1. Vat photopolymerization (VPP)

The VPP process is an AM technology based on a liquid photosensitive resin, which is cured layer by layer using a light source, resulting in a solid 3D part. Several variations of VPP exist, including stereolithography, digital light processing, two-photon polymerization, and volumetric 3D printing.[11] Commonly employed light sources include laser, digital light projection, and LED systems, offering varying resolutions and processing speeds.[12] VPP is capable of achieving micron- to nanometer-scale resolution, making it well-suited for manufacturing components requiring high dimensional accuracy and superior surface quality.[13] This technique has been widely applied

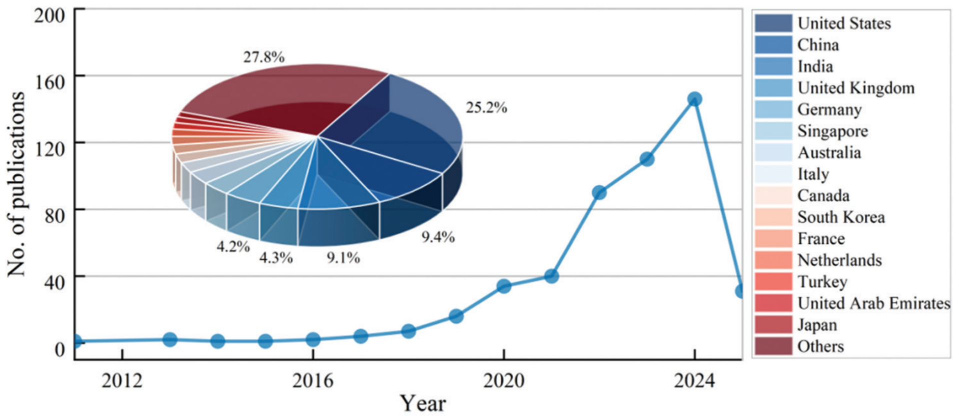

Figure 1. Research and development trends are reflected by the number of publications in the field of machine learning for material design of AM (data acquired from the Scopus database)

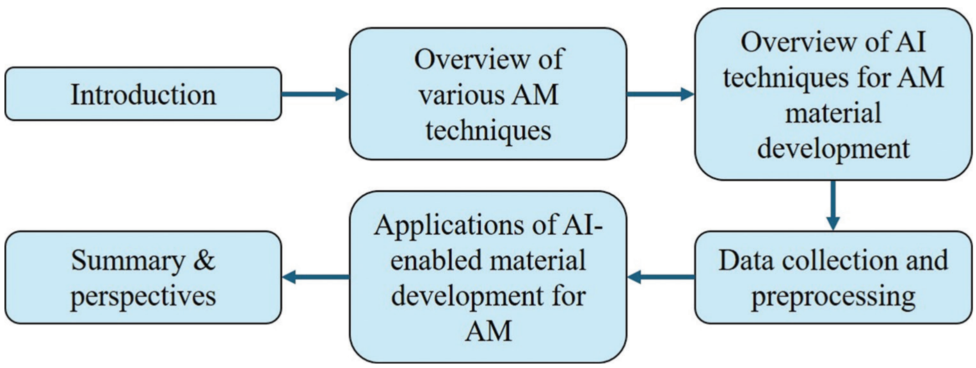

Figure 2. The framework of this work
Abbreviations: AI: Artificial intelligence; AM: Additive manufacturing.

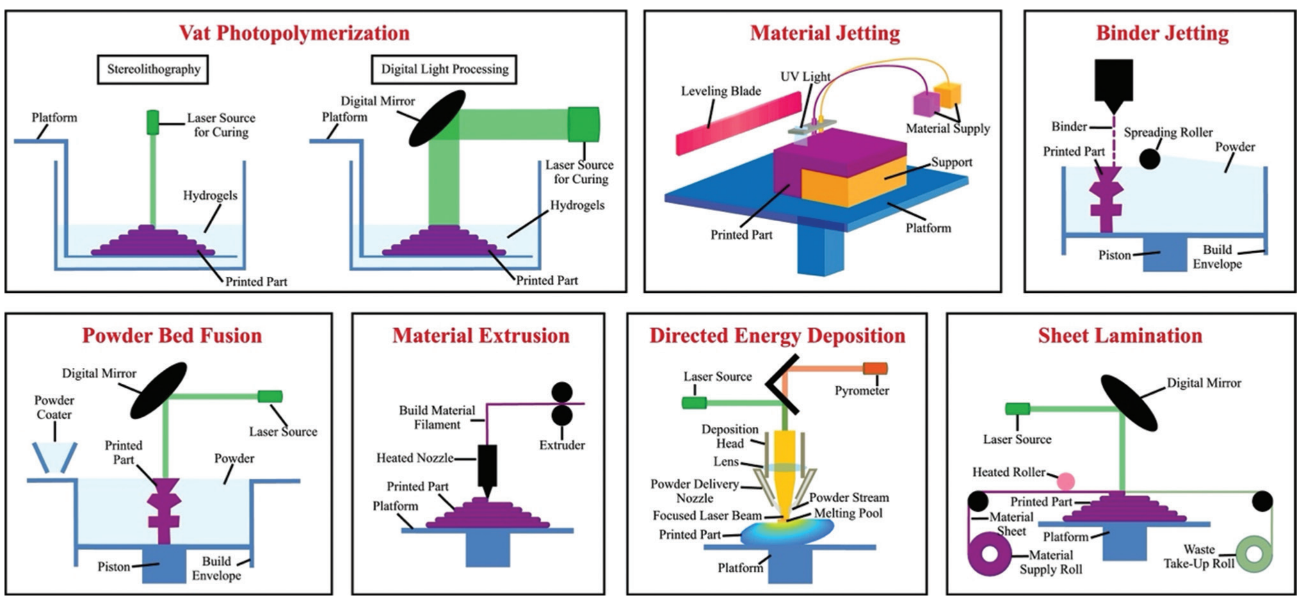

Figure 3. Categories of additive manufacturing techniques. Reproduced from Jin *et al.*[10]

in industrial engineering, regenerative medicine, smart materials, and both nano- and micro-scale manufacturing. It also holds significant promise for emerging applications such as 4D printing and bioprinting.[12]

2.2. Material jetting (MJT)

MJT operates similarly to inkjet printing, where liquid materials are deposited as microdroplets through a print head and cured by ultraviolet light to build a structure.[14] The process utilizes two types of materials: Build material, which forms the final part, and support material, which provides structural integrity during printing and is later removed through dissolution. MJT technology has the advantages of high resolution, multi-material printing capability,[15] and the ability to fabricate intricate geometries, surpassing material extrusion (MEX), binder jetting (BJT), and powder bed fusion (PBF) in surface accuracy.[16] It is widely applied in aerospace, biomedical, dental, and mechanical engineering.[16]

2.3. BJT

BJT constructs 3D structures by selectively depositing a liquid binder onto a powder bed, gradually bonding the material to form the desired shape. Unlike other AM methods, BJT does not require a heat source, such as a laser or electron beam, making it a more cost-effective approach.[17] BJT-printed parts are self-supporting, eliminating the need for support structures and enabling the simultaneous fabrication of multiple components.[13] However, the printed parts often exhibit lower mechanical strength, necessitating post-processing treatments, such as sintering or infiltration, to improve material performance.[13] BJT is widely applied in biomedical engineering,[18] mold casting,[19] and food technology.[20]

2.4. PBF

PBF is a widely adopted AM process, primarily used for metals[21] and polymers,[22] with limited applications in ceramics and composites.[13] It has several different terms, including selective laser sintering, electron beam melting, selective laser melting, and direct metal laser sintering. PBF utilizes a powder bed, where the material is selectively fused using a laser or electron beam, with layer deposition and fusion repeating until the final structure is formed. An inert gas-protective environment is often needed to prevent oxidation.

Despite its widespread use, materials used for PBF still primarily derive from commercially available materials, which were not originally designed for AM, leading to several key challenges.[23] Many existing commercial alloys (e.g., 7075Al alloy, H13 tool steel, Inconel718 nickel-based superalloy, and CoCrFeMnNi Cantor high-entropy alloy) are prone to hot cracking and defect formation, compromising part integrity and limiting their applicability. In addition, controlling microstructure evolution remains a critical issue, as rapid solidification and complex thermal histories have a critical influence on grain structure, dislocation evolution, and phase transformation behavior. To overcome these limitations, advancements in AM-specific material development are essential to optimize phase stability, enhance mechanical properties, and, in particular, ensure reproducibility.

2.5. Material extrusion

In MEX, a material is first heated to its melting point, then extruded as a filament, and finally deposited to form a structure. Two common MEX methods include fused deposition modeling (FDM) and direct ink writing (DIW). FDM relies on thermoplastic filaments that are melted and extruded, making it widely used for rapid prototyping, educational applications, and engineering part fabrication due to its low cost, ease of handling, and ability to print with multiple materials. In contrast, DIW involves extruding high-viscosity inks, pastes, or gels, enabling the fabrication of soft materials, ceramics, and bioprinted structures. Due to its low cost, ease of handling, and capability for multi-material printing, MEX is well-suited for rapid prototyping, educational applications, and engineering part fabrication.[13] However, its relatively low resolution limits its suitability for small-scale or highly detailed components. At present, the MEX process is widely used in medical modeling, engineering parts, prototyping, tissue engineering, and bioprinting devices.[24]

2.6. Directed energy deposition (DED)

DED melts and deposits materials simultaneously using a high-energy heat source, such as a laser beam or arc.[13] The process utilizes powder or wire as feedstock, with material introduced into a molten pool during printing. Multi-axis motion control enables complex geometries, making DED suitable for metallic multi-materials, functional gradient materials, composite fabrication, and component repair.[25] Notably, DED is primarily used for metallic materials and offers a significantly higher deposition rate than PBF, making it favorable for large-format component fabrication.

Despite its versatility, DED material design remains complex because the rapid solidification leads to non-equilibrium microstructures, affecting phase stability, residual stress, and mechanical performance.[25] Similar to PBF, most alloys used in DED are legacy alloys originally designed for conventional manufacturing methods, limiting the full exploration of DED's potential. This underscores the critical need for developing AM-specific materials to fully leverage the capabilities of these AM techniques.

2.7. Sheet lamination (SHL)

SHL constructs 3D parts by stacking and bonding material layers, which are cut using laser or mechanical cutters. The process follows two main approaches: Bond-then-form and form-then-bond.[13] Compared to other AM techniques, SHL offers cost-effective material usage and rapid processing, making it particularly suited for large and thick components.[26] In addition, SHL does not require support structures, enabling the fabrication of complex geometries directly.[26] SHL has also shown various applications in aerospace,[27] automotive,[28] medical,[29] and bioengineering fields.[30]

3. Overview of AI techniques for AM material development

The advancement of AI has significantly influenced traditional manufacturing, enhancing the productivity, efficiency, and flexibility of AM.[31] This section explores three major categories of AI techniques for material development, analyzing their applications in materials development, as illustrated in Figure 4. Table 1 summarizes the common AI methods employed across different stages of AM, including their typical applications, strengths, and limitations.

3.1. Machine learning (ML)

ML, a subset of AI, is primarily categorized into supervised learning, unsupervised learning, and reinforcement learning, enabling computers to learn from data without explicit programming.[32] Common ML methods include k-nearest neighbor and support vector machine.

ML has been increasingly applied to conventional materials development. For example, Dang *et al.*[33] used the support vector regression model to predict the fatigue life of titanium alloys by analyzing their microstructural characteristics, including the stress intensity near the holes and the type of holes. Besides, Ling *et al.*[34] used the

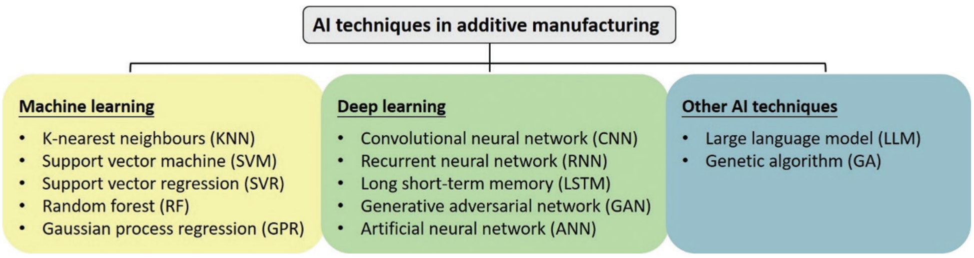

Figure 4. Categories of AI techniques in additive manufacturing
Abbreviation: AI: Artificial intelligence.

Table 1. Summary of common AI methods, applications, strengths, and limitations across key AM steps

AM steps	Common AI methods	Typical applications	Strengths	Limitations
AM design	RF, SVM, NNs, Lasso/elastic net regression, GA, feed-forward NN, Bayesian inference, hierarchical clustering	Feature recommendation, part mass, and cost prediction, build time estimation, topology design, thermal compensation, shape deviation prediction	RF is robust to noisy data; SVM is effective with small datasets; GA enables global search; NNs capture complex non-linear relations	NNs require large datasets and long training; SVMs are sensitive to kernel settings; GA can be time-consuming; RF may bias toward dominant features
AM process and performance optimization	Back propagation NN, SOM, LS-SVM, GPR, Kriging, GA	Melt pool depth/width prediction, powder spreading, strength/hardness estimation, porosity and density prediction	NNs capture complex non-linearities; GPR provides uncertainty quantification; GA is good for multi-objective optimization	GPR scales poorly; NNs are data-hungry; GA performance depends on parameter tuning
In situ process monitoring and control	NN, SVM, Naive Bayes clustering, CNNs, deep belief networks (deep learning), K-means	Porosity and defect detection, anomaly detection, spatter classification, acoustic emission analysis, multi-sensor fusion, CT-aided defect identification	Probabilistic models handle uncertainty; CNNs/deep belief networks are excellent for sensor/image data; clustering helps early-stage pattern recognition	Deep models are computationally demanding; clustering accuracy may be low; Naive Bayes assumes feature independence
Testing and validation	Sparse representation, KNN, Naïve Bayes clustering, SVM, decision trees	Point cloud-based dimensional analysis, defect classification (e.g., porosity)	KNN is simple and intuitive; SVMs are robust; sparse models are suited to high-dimensional data	KNN suffers in high dimensions; decision trees overfit easily; sparse models require careful tuning

Abbreviations: CNN: Convolutional neural network; CT: Computed tomography; GA: Genetic algorithm; GPR: Gaussian process regression; KNN: K-nearest neighbor; NNs: Neural networks; LS-SVM: Least squares support vector machine; RF: Random forest; SOM: Self-organizing map; SVM: Support vector machine; AI: Artificial intelligence; AM: Additive manufacturing.

random forest (RF) algorithm to predict the fatigue life of a steel sample by analyzing a fatigue test dataset of 439 steels containing nine alloying elements, and from the 437 possible combinations to select the composition and treatment of steel with the best fatigue life. In addition, Navarrete *et al.*[35] used ML models to predict the static yield stress of mixed cement pastes containing supplementary cementitious materials by collecting datasets from previous experimental work, and have compared the prediction accuracies of different ML models, including multilayer perceptron, RF, and support vector regression.

These studies, although not related to AM, have demonstrated the capabilities of ML in material property prediction and process optimization. By extracting complex relationships from extensive experimental datasets, ML models improve decision-making, process efficiency, and reliability. As ML techniques continue to evolve, their integration with computational modeling and experimental validation will further accelerate the design of next-generation materials and enhance manufacturing intelligence.

3.2. Deep learning (DL)

DL leverages multilayer neural networks to extract features, identify patterns, and model complex relationships in high-dimensional data.[36] Compared to traditional ML methods, DL excels in automatic feature learning, making it particularly effective for image-based analysis, sequential data modeling, and generative design. Common DL architectures include convolutional neural networks (CNNs), recurrent neural networks, long short-term memory, generative adversarial networks (GANs), and artificial neural networks (ANNs).

DL extends data-driven approaches in material development, playing a key role in microstructure-property correlation, process design, and automated material discovery. For example, Gu *et al.*[37] used DL for the design of layered materials and trained a finite element analysis (FEA) model to obtain high-performance materials. Specifically, CNN was used to predict the mechanical properties of composites and combined it with a self-learning algorithm to optimize the design of the materials. Li *et al.*[38] investigated the joint effects of the size, depth, distribution, and orientation of defects on the fatigue life of AM-built Ti-6Al-4V alloys by constructing an ANN-based model, revealing how these factors interact with each other, which in turn affects the durability of the Ti-6Al-4V alloy. Shen and Buehler[39] developed a novel unsupervised GANs (specifically StyleGAN) approach, trained with input unlabeled data, to construct a latent space that is free to be explored for material design without human intervention. Lee *et al.*[40] used the GAN model to generate additional data to solve the problem of insufficient samples, which successfully improved the accuracy of the phase prediction of high-entropy alloys and revealed the key design parameters, providing a new insight for the design and discovery of high-entropy alloys.

3.3. Other AI techniques

Large language models (LLMs) are a class of AI models extensively applied in natural language processing. LLMs capture complex linguistic patterns and structures, enabling multilingual processing and contextual understanding. Their capabilities extend beyond language applications, with emerging studies demonstrating their potential in materials science and engineering. For example, Buehler[41] developed MechGPT, an LLM-based framework designed to simulate and analyze mechanical behavior and failure mechanisms, improving the predictive accuracy of material properties and supporting the design of novel materials.

Genetic algorithms (GA) provide an effective strategy for global optimization, employing selection, mutation, and crossover to explore complex solution spaces. In the study of Shen and Buehler,[39] they used GA to further optimize the microstructure of the model-designed materials to improve their mechanical properties. Nazar *et al.*,[42] on the other hand, combined GA with the gene expression concept to develop a new gene expression programming model to predict the plastic viscosity and yield stress of fresh concrete used for the MEX process by analyzing six key factors, such as cement, sand, water, different sizes of coarse aggregate, and superplasticizers, to improve the accuracy and efficiency of predicting the rheological parameters of concrete.

4. Data collection and pre-processing

A typical workflow of AI-driven material development in AM is illustrated in Figure 5. The workflow begins with the collection of raw data from various sources, such as simulations, experiments, literature, and databases. The raw data undergoes pre-processing to refine it for AI applications. Subsequently, AI algorithms are applied to train models that predict material behavior or suggest optimal material compositions. The workflow iteratively integrates feedback from experiments and simulations to refine the dataset and improve prediction accuracy.

Data collection and pre-processing are fundamental to the successful implementation of this workflow. High-quality and comprehensive datasets enable AI models to identify underlying correlations and outliers that would be difficult to discern through traditional analysis. However, the heterogeneity and complexity of data sources –

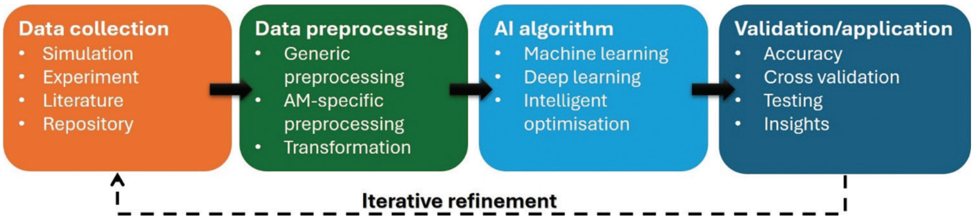

Figure 5. Workflow for artificial intelligence-driven material development in additive manufacturing

ranging from atomic-scale simulations to experimental measurements – present significant challenges. These challenges include inconsistencies in data formats, missing and noisy values, and variability in measurement techniques. Pre-processing mitigates these issues by standardizing and transforming raw data, ensuring its compatibility with AI algorithms.

4.1. Data collection

Data for material development are primarily derived from simulations and/or physical experiments. Overall, the types of datasets for material development can be broadly categorized into scalar, time-series, spectral, image, categorical, and spatial data. Scalar data represents single-value material properties, such as tensile strength and elastic modulus. Time-series data captures changes over time, such as stress-strain behavior during tensile testing. Spectral data reveals material composition and structure through techniques, such as X-ray diffraction. Image data mainly includes microstructure images, while categorical data describes qualitative attributes, such as phase and defect types. Spatial data represents geometries and positional relationships, including crystallographic texture. Table 2 summarizes the common types of data obtained through simulations and experiments.

Simulation plays a critical role in AI-driven material development by providing high-fidelity datasets that capture complex material behaviors and properties. These simulations are favorable for generating datasets that can support predictive modeling and validate AI-driven solutions. Commonly employed modeling methods include density functional theory (DFT), FEA, and computer coupling of phase diagrams and thermochemistry (CALPHAD). DFT is widely used for predicting electronic structures and thermodynamic properties. FEA focuses on macroscopic phenomena, such as stress-strain behavior and thermal conductivity under various conditions. CALPHAD, on the other hand, is instrumental in phase diagram calculations and thermodynamic modeling. Complementing simulation, experimental measurements provide essential data that capture the real-world behavior and performance of materials. These measurements not only validate simulation results but also offer unique empirical insights. Common techniques include property testing, microscopy, and spectroscopy.

Table 2. Common data types and sources in material development

Data source	Data type	Examples
Experiment	Scalar	Ultimate tensile strength, hardness, relative density, and thermal conductivity
	Time-series	Stress-strain curve and thermography
	Spectral	X-ray diffraction, X-ray dispersive spectroscopy, X-ray photoelectron spectroscopy, and Raman spectroscopy
	Image	Scanning electron microscopy, transmission electron microscopy, and atomic force microscopy
	Categorical	Phase and defect
	Spatial	Crystallographic texture, pore distribution, and filler dispersion
Simulation	Scalar	Total energy (DFT), Gibbs free energy (CALPHAD), elastic modulus (DFT, FEM), and stress/strain (FEM)
	Time-series	Displacement evolution (FEM)
	Spectral	Density of states (DFT)
	Image	Charge density maps (DFT) and stress/strain field (FEM)
	Categorical	Phase regions (CALPHAD) and failure regions (FEM)
	Spatial	Atomic position (DFT)

Abbreviations: CALPHAD: Calculation of phase diagrams; DFT: Density functional theory; FEM: Finite element method.

In material development for AM, datasets are often sourced from literature, online databases, or experiments.[43] Table 3 summarizes the commonly used online data repositories. While online material databases provide valuable resources for material development, most existing repositories are primarily built upon data obtained through traditional manufacturing processes. Key aspects of AM, such as the rapid solidification, residual stresses, and complex microstructural evolution characteristics, are typically not captured. As a result, applying data from these repositories directly to AM may lead to inaccuracies,

Table 3. Online repositories of materials

Name	Description	Material	Source	Availability
AFLOWLIB.ORG[44]	High-throughput computational database for material properties, focusing on thermodynamics and electronic structures	Metals	DFT	http://aflow.org/(Free access)
Alloy database	Focused on structure and enthalpy of formation for alloy systems, including stable and metastable phases	Metals	DFT	http://alloy.phys.cmu.edu/(Free access)
ASM database	Comprehensive database on material properties, phase diagrams, and processing data	Metals, polymers	Experiment, CALPHAD	https://www.asminternational.org/(License required)
CINDAS LLC	Provides critically evaluated databases for thermal, mechanical, electrical, and physical properties of materials, including aerospace alloys	Metals	Experiment	https://cindasdata.com/(License required)
Computational materials repository	Open platform for accessing materials property datasets derived from simulations, including thermodynamic and mechanical properties	Metals	DFT, MD	https://cmr.fysik.dtu.dk/(Free access)
Crystallography open database[45]	Open-access collection of crystal structures of organic, inorganic, metal-organic compounds, and minerals	Metals	Experiment	http://www.crystallography.net/(Free access)
Inorganic crystal structure database[46]	Curated database of crystallographic data for inorganic compounds; provides high-quality structural information for metals, ceramics, and minerals, with additional crystallographic parameters calculated	Metals	Experiment	https://icsd.fiz-karlsruhe.de/(License required)
Joint Automated repository for various integrated simulations[47]	Comprehensive platform supporting the Materials Genome Initiative, designed to accelerate materials discovery for energy, electronics, and mechanical applications	Metals, polymers	DFT, MD, experiment	https://jarvis.nist.gov/(Free access)
Knovel database	Engineering materials database covering properties, such as mechanical strength, thermal stability, and chemical behavior	Metals, polymers	Experiment	https://app.knovel.com/(License required)
Matmatch	Interactive platform designed for material selection, offering comprehensive datasets on material properties and enabling comparisons for engineering and design applications	Metals, polymers	Experiment	https://matmatch.com/(Free access)
Materials-cloud[48]	Open-access platform for computational materials science, serving as a "repository of repositories" similar to GitHub; provides data sharing, simulation workflows, and educational resources to support reproducibility and collaboration	Metals	DFT	https://www.materialscloud.org/(Free access)
MatNavi	Comprehensive materials database platform featuring sub-databases for polymers (chemical structures, processing properties, and NMR spectra), inorganic materials (crystal structures, phase diagrams, and physical properties), metallic materials (density, elastic constants, and creep characteristics), and computational electronic structure data (band structures from first-principles calculations)	Metals, polymers	Experiment, CALPHAD, DFT	https://mits.nims.go.jp/(Free access)
MatWeb	Searchable database providing detailed material property data for a wide range of engineering materials	Metals, polymers	Experiment	http://www.matweb.com/(Free access)

(Cont'd...)

Table 3. *(Continued)*

Name	Description	Material	Source	Availability
NIST DATA	Comprehensive repository offering experimental and computational material property data, including phase diagrams, thermophysical properties, and structural information	Metals, polymers	DFT, CALPHAD, MD, Monte Carlo, FEA, experiment	https://www.nist.gov/data/ (License required for some datasets)
NOMAD repository[49]	Platform for computational materials science providing FAIR (Findable, Accessible, Interoperable, Reusable) data sharing; includes the world's largest repository of computational raw data, normalized into a code-independent format, enabling data mining and machine learning for materials discovery	Metals	DFT	https://nomad-lab.eu/(Free access)
NREL MatDB	Computational materials database with a specific focus on materials for renewable energy applications, including, but not limited to, photovoltaic materials, materials for photo-electrochemical water splitting, and thermoelectric	Metals	DFT	https://materials.nrel.gov/ (Free access)
OpenKIM[50]	Curated repository of interatomic potentials and analytics for making classical molecular simulations of materials reliable, reproducible, and accessible	Metals	DFT, experiment	https://openkim.org/(Free access)
Predictive integrated structural materials science	Repository combining materials science data, models, and workflows to support advanced simulations	Metals	DFT, CALPHAD, experiment	http://www.prisms-center.org/(Free access)
The materials project[51]	Open-access platform for computational materials science that uses high-throughput calculations to compute and disseminate properties of materials; provides structural, electronic, and thermodynamic properties for accelerating materials discovery and design	Metals	DFT	https://materialsproject.org/ (Free access)
Total material	Comprehensive materials information platform providing access to data on over 540,000 metallic and non-metallic materials; includes extensive mechanical and physical property data, global standards and equivalencies, stress-strain, and fatigue properties	Metals, polymers	Experiment	https://www. totalmateria.com/(License required)
The open quantum materials database[52]	High-throughput database containing over 200,000 DFT calculations of crystal structures and formation energies; serves as a resource for materials discovery, providing thermodynamic stability analysis, chemical potential data, and datasets for training machine learning models	Metals	DFT	https://oqmd.org/(Free access)

Abbreviations: CALPHAD: Calculation of phase diagrams; DFT: Density functional theory; FEA: Finite element analysis; MD: Molecular dynamics.

particularly when predicting material performance under AM-specific conditions. However, these traditional datasets can still serve as initial guidance for material selection and composition screening. By integrating such data with AM-specific experimental results and process parameters (e.g., laser power, scan speed, and cooling rates), AI models can be adapted to better reflect the unique processing-structure-property relationships in AM. Developing specialized AM databases that incorporate both material composition and AM process conditions remains an essential step for advancing AI-driven material development in this field.

4.2. Data pre-processing

Data pre-processing is for ensuring that raw data are systematically refined into a structured format suitable for computational analysis and model training. Given the inherent imperfections in raw datasets, such as noise, inconsistencies, and incomplete records, pre-processing plays a crucial role in mitigating these issues. The presence of unprocessed data can significantly compromise the accuracy and reliability of AI models, necessitating robust pre-processing methodologies to enhance data quality and ensure compatibility with ML algorithms. A well-designed pre-processing pipeline ensures that datasets are not only internally consistent but also scalable and representative of the underlying material properties and behaviors. Furthermore, it facilitates bias mitigation, minimizes redundancy, and enhances predictive accuracy.

4.2.1. Fundamental data pre-processing techniques

Data pre-processing typically begins with data cleaning, a process that involves handling missing values, detecting and correcting inconsistencies, and eliminating outliers. In AI-based material research, missing values can arise from incomplete experimental records or sensor failures during process monitoring. Various imputation strategies can be applied depending on data type and structure. For numerical variables, mean or median imputation is commonly used, whereas categorical data are often addressed using the most frequent category or probabilistic imputation techniques[53]

Feature encoding is another critical step, particularly when dealing with categorical attributes, such as material compositions, process parameters, and classification labels. Conventional encoding techniques, such as one-hot encoding, enable categorical variables to be represented numerically without introducing unintended ordinal relationships. Feature scaling follows as a necessary step to ensure comparability across different feature dimensions. Common approaches include min-max normalization, which scales features to a defined range, and standardization (Z-score normalization), which transforms features to have zero mean and unit variance, mitigating the effects of disproportionate feature magnitudes on model training.

4.2.2. Pre-processing strategies for data in AM

Unlike conventional structured datasets, datasets in AM are inherently multimodal, encompassing tabular datasets, high-resolution imaging, time-series process data, and three-dimensional geometric representations. As a result, pre-processing strategies must be adapted to accommodate these diverse data formats while ensuring cross-modality compatibility.

One of the key challenges in AM data pre-processing is data registration, which aligns information obtained from different stages of the manufacturing process. For example, ensuring that *in situ* monitoring data is correctly mapped to corresponding microstructural characterization results is essential for accurate process–property correlations. This alignment is particularly relevant in AM, where variations in process parameters directly influence material structure and mechanical performance.

In addition, AM datasets are often structured across multiple spatial and temporal scales. Multiscale data integration is necessary to harmonize information collected at different levels, such as individual powder particles, melt pools, printed layers, and entire components. This requires the standardization of spatial resolutions and temporal sampling rates to enable meaningful feature extraction and pattern recognition.

Feature extraction is a particularly critical aspect of pre-processing in AM, as raw sensor data often requires transformation before it can be effectively utilized in AI models. For example, three-dimensional data derived from X-ray, computed tomography (CT) scans,[54] or microstructure imaging may be converted into structured representations through voxelization. Similarly, time-series data from thermal sensors or acoustic emission monitoring may be analyzed using the Fourier[55] or Wavelet[56] transforms to extract frequency-based features relevant to defect detection and process stability. Dimensionality reduction techniques, such as principal component analysis, are frequently applied to condense high-dimensional feature sets while preserving essential information.[57]

5. Applications of AI-enabled material development for AM

The development of materials with optimized properties is a central objective, driving advancements in structural, functional, and high-performance materials. The pursuit of improved mechanical strength, thermal stability, electrical conductivity, and biocompatibility has led to extensive research into metals, polymers, and bioinks/biomaterial inks.

This section explores the applications of AI in material development for AM, with a particular focus on metals, polymers, and bioinks/biomaterial inks. For metals and polymers, the discussion is structured into two key aspects: Material design and performance optimization. In the material design section, we examine how AI-driven methods facilitate the discovery and optimization of novel compositions/structures tailored for AM processes. The performance optimization section extends this analysis by establishing a link between AM process parameters and material performance (Figure 6), leveraging AI to refine microstructural features and mechanical properties. For bioinks and biomaterial inks, the focus is on AI-assisted formulation optimization, where balancing printability, rheological properties, biocompatibility, and mechanical integrity is crucial for ensuring successful bioprinting outcomes.

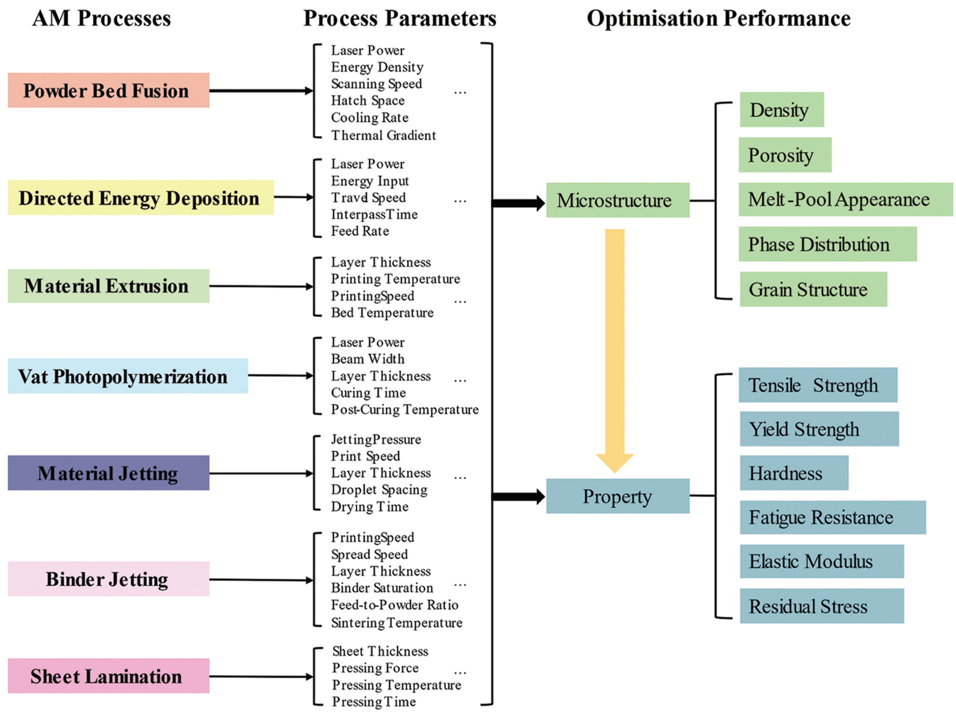

Figure 6. Link between additive manufacturing process parameters and material microstructure and properties. Adapted from Jin *et al.*[10]

5.1. Metallic materials for AM

Table 4 presents a summary of AI applications related to metal materials in AM. The following sections will explore representative examples to elucidate how AI facilitates material design and performance optimization.

5.1.1. Alloy design for metal AM

A prominent success of AI-driven alloy design is its application in phase prediction for high-entropy alloys. Due to their multi-principal element nature, high-entropy alloys exhibit a vast range of possible phase structures, which directly influence their mechanical, thermal, and chemical properties.[67] A variety of ML models have been employed to classify high-entropy alloy phases, employing diverse feature sets to improve prediction accuracy. Commonly used models include ANNs,[68-70] RF,[71,72] support vector machine,[73,74] logistic regression,[75] gradient-boosted trees,[76] and Gaussian process classification.[77] These models utilize input features, such as atomic size difference (δ), valence electron concentration, mixing enthalpy (H_{mix}), and entropy parameters, to predict phase formation, including face-centered cubic, body-centered cubic, hexagonal close-packed, and multiphase structures.

Beyond high-entropy alloys, AI has also been employed to optimize the composition of green maraging steels for AM. As seen in Figure 7, Tan *et al.*[58] employed ML algorithms to optimize the composition of Fe–Ni–Ti–Al maraging steel, tailoring it for AM. Specifically, this study utilized thermodynamic simulations to generate a dataset, which was subsequently integrated with RF, decision trees, AdaBoost, and k-nearest neighbor to predict the formation of Ni_3Ti precipitates and Laves phases during AM. Based on these predictions, the concentrations of Ni, Ti, and Al were adjusted to enhance precipitation strengthening while mitigating the formation of detrimental phases, thereby improving microstructural stability and mechanical properties. Finally, the newly developed maraging steel exhibits exceptional mechanical properties, achieving a tensile strength of 1,538 MPa and a uniform elongation of 8.1%, validating the effectiveness of the AI-driven material development approach.

Overall, while AI-driven methodologies have demonstrated significant potential in alloy design, the direct application of AI in AM-specific alloy design is still rare. Most studies still focus on general material design, where AI is primarily employed for composition optimization[78] and phase prediction,[79] without explicitly considering the constraints imposed by AM processing. To enhance the applicability of AI-driven alloy design for AM, it is essential to further integrate it with process-aware models that account for rapid solidification, thermal cycling, and process-induced defects.

Table 4. Summary of AI applications for metal materials for AM

AM process	Material	Optimization type	AI method	Target	Model performance	References
DED	Fe–Ni–Ti–Al	Design	RF	Composition optimization	R2=0.998 MAE=0.292	Tan *et al.*[58]
PBF	SS316L	Performance	Adaptive Neuro-Fuzzy Inference System (ANFIS)	Fatigue life prediction	RMS=14.66%	Zhang *et al.*[59]
PBF	Zr52.5Cu17.9Ni14.6Al10Ti	Performance	HGP	Materials characteristics prediction	RMSE=2.58%	Chernyavsky *et al.*[60]
PBF	AlSi10Mg	Performance	GPR	Tensile property optimization (YS and elongation)	-	He *et al.*[61]
PBF	AlSi10Mg	Performance	GPR	Density variations and microstructural characteristics prediction	-	Liu *et al.*[62]
PBF	Ti-6Al-4V	Performance	MML	Fatigue strength design	-	Awd *et al.*[63]
PBF	Ti-6Al-4V	Performance	ANN	Tensile property optimization (YS, UTS, and elongation)	R2: YS=0.9887, UTS=0.9921, elongation=0.9917	Maleki *et al.*[64]
PBF	Ti-6Al-4V	Performance	RSM+GA	Energy absorption optimization	R2=0.9431	Meng *et al.*[65]
DED	Ti–Mn alloy	Performance	GPR	YS and modulus optimization	MAPE: YS=6.26%, E=2.02%	Gong *et al.*[66]

Abbreviations: ANN: Artificial neural networks; DED: Directed energy deposition; E: Elastic modulus; GA: Genetic algorithms; GPR: Gaussian process regression; HGP: Heteroscedastic Gaussian process; MAE: Mean absolute error; MML: Mechanistic machine learning; PBF: Powder bed fusion; RF: Random forest; RMS: Root mean square; RMSE: Root mean square error; RSM: Response surface methodology; UTS; Ultimate tensile strength; YS: Yield strength; AI: Artificial intelligence; AM: Additive manufacturing.

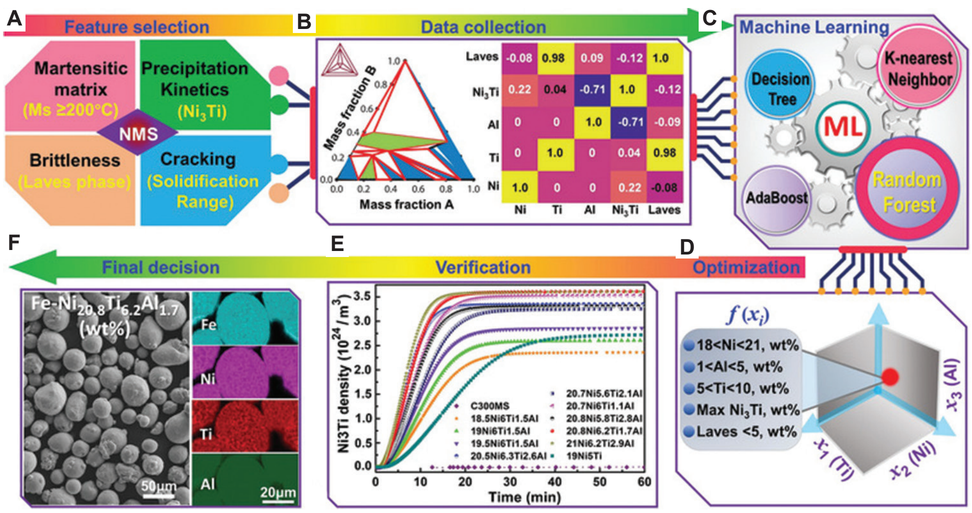

Figure 7. The schematic of ML-assisted composition design of Fe–Ni–Ti–Al NMS. (A) Feature selections in the design of NMS. (B) Data collections from Thermo-Calc software and the correlation matrix of the input composition (Ni, Ti, and Al) and output (Ni_3Ti precipitate and Laves phase weight fractions) in the surrogate models. (C) ML by various algorithms (random forest is the most accurate one). (D) Composition optimization for the allowable range of alloying elements. (E) Time-dependent dynamic precipitation behaviors of different compositions at 490°C (the balance is Fe). (F) Optimal composition Fe-20.8Ni-6.2Ti-1.7Al (wt%) along with the morphology and elemental mapping of the produced powder. Reproduced from Tan *et al.*[58]
Abbreviations: NMS: Novel maraging steel; ML: Machine learning.

5.1.2. Performance optimization in metal AM

Alloy performance optimization includes both microstructural optimization and mechanical property optimization. Microstructural optimization focuses on the regulation of grain size, phase distribution, precipitate morphology, and porosity to achieve improved structural homogeneity and stability. Mechanical property optimization, on the other hand, primarily focuses on the enhancement of properties, including strength, hardness, ductility, and fracture toughness, which are typically realized through appropriate microstructural and process control.

Recent advancements in AI-driven methodologies have enabled the establishment of correlations between processing parameters and microstructural characteristics in AM. By leveraging ML models trained on experimental and computational datasets, AI enables more accurate predictions of microstructural evolution and mechanical properties under varying process conditions. For example, Awd *et al.*[63] integrated mechanistic ML with physics-based models to predict and optimize the fatigue strength of AM-fabricated metamaterials. Their approach combines electronic structure calculations, stochastic process modeling, and microstructural characterization to establish process-structure-property (PSP) relationships. Through μ-CT imaging and defect quantification, they demonstrated how AI-driven methodologies can enhance fatigue damage modeling, enabling more accurate predictions of material performance under cyclic loading. Similarly, Liu *et al.*[62] employed Gaussian process regression (GPR) to model the complex relationships between processing parameters, microstructure, and mechanical properties in laser powder bed fusion (LPBF)-fabricated AlSi10Mg. GPR was utilized to predict density variations and microstructural characteristics based on key process parameters. Their study demonstrated that GPR effectively captures non-linear dependencies within PSP relationships, allowing for improved process parameter selection to minimize defects and enhance mechanical performance. The model showed strong agreement with experimental results, suggesting reliable prediction accuracy.

In addition, Gaussian process-based models have been explored to optimize process parameters for improved mechanical performance. Tapia *et al.*[80] developed a Gaussian process-based surrogate modeling framework to predict melt pool depth in LPBF of 316L stainless steel, thereby identifying processing windows that enhance part quality. Their approach enabled the classification of conduction-mode and keyhole-mode melting regimes, which directly affect the microstructure and, consequently, the mechanical properties of AM components. Chernyavsky *et al.*[60] introduced a Heteroscedastic Gaussian process (HGP) model to predict the amorphicity of a Zr-based glass-forming alloy fabricated through LPBF. This model effectively establishes a quantitative link between LPBF conditions and microstructural evolution. Figure 8 illustrates the predictive capability of the HGP model, covering amorphicity distribution (Figure 7A), uncertainty quantification (Figure 7B), and prediction accuracy (Figure 7C). These results highlight the model's robustness in not only delivering accurate amorphicity predictions but also in assessing dataset reliability and identifying underlying physical mechanisms governing glass formation in AM.

The integration of AI-driven methodologies in alloy performance optimization has significantly advanced the understanding and prediction of PSP relationships.

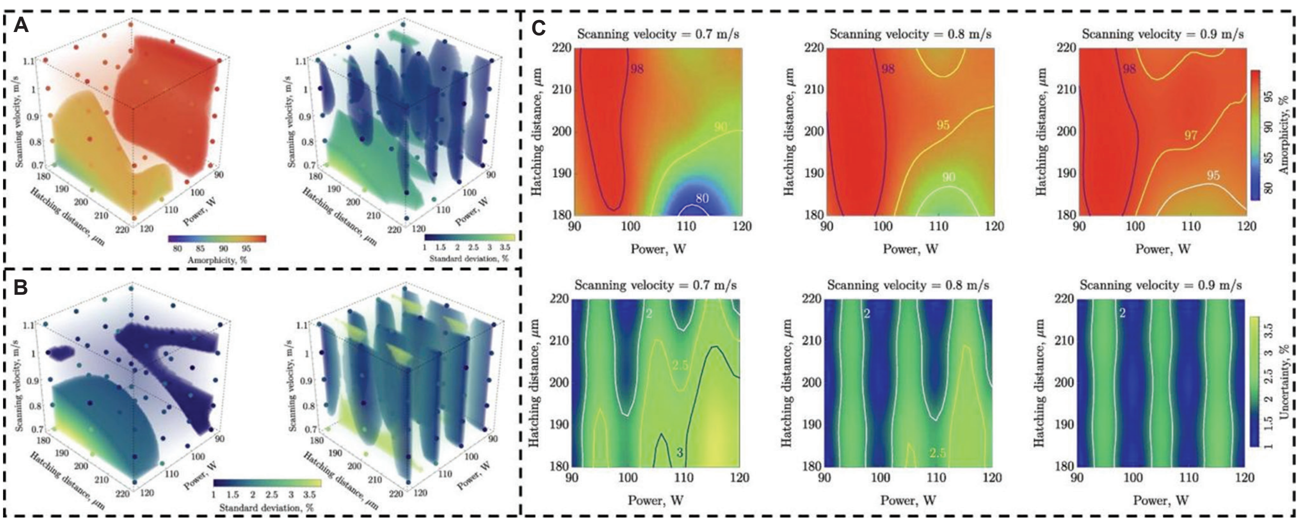

Figure 8. Predicted amorphicity distributions and associated uncertainty for alloys fabricated through laser powder bed fusion. (A) HGP model predictions for mean values of amorphicity and its total uncertainty. (B) Position-resolved aleatoric and epistemic uncertainties predicted by the HGP model. (C) Two-dimensional contour maps of HGP model predictions for mean values of amorphicity and its total uncertainty. Reproduced from Chernyavsky *et al.*[60]
Abbreviation: HGP: Heteroscedastic Gaussian process.

From fatigue strength modeling to process parameter optimization, AI has proven to be a powerful tool in enhancing microstructural control and mechanical property refinement. Despite these advancements, challenges remain in data completeness, model interpretability, and generalization across different AM processes and material systems. The continued development of hybrid AI approaches, integrating physics-based models with data-driven learning, will be essential for further improving predictive accuracy and expanding the applicability of AI in AM alloy design.

5.2. Polymer materials for AM

Table 5 compiles a range of AI-driven strategies applied to polymer AM, covering both compositional design and property improvement.

Table 5. Summary of artificial intelligence applications for polymer materials for additive manufacturing

AM process	Material	Optimization type	AI method	Target	Model performance	References
PBF	Multi-material	Design	GMM and PCR	Elastic property optimization	Poisson's ratio error≈16%	Chen *et al.*[81]
VPP	RPU+SilDN	Design	VAE and BO	Elastic moduli tailoring (Young's modulus and Poisson's ratio)	Poisson's ratio error≈6.4%, E error≈11.3%	Xue *et al.*[82]
VPP	TPU	Design	MLP	Novel metamaterial with variable compression properties design	-	Fleisch *et al.*[83]
MET	PLA	Performance	Bayesian ML	Super-compressibility and recoverability design	R2≈0.988	Bessa *et al.*[84]
MET	PLA	Performance	RF, KNN, ADA, DT, and LSTM	Tensile and flexural strength prediction and optimization	LSTM achieved best performance: R^2=0.9169, MAPE=2.85%, RMSE=2.44; other models (RF, KNN, ADA, DT) showed R^2 <0.75 and MAPE >5%.	Sharma *et al.*[85]
MET	Technomelt PA 6910	Performance	LiR, GPR, RR, and KNN	Tensile property prediction (Young's modulus, yield stress, yield strain, tensile stress, and tensile strain)	LiR/RR best: <10% error	Nasrin *et al.*[86]
MET	ABS	Performance	LiR, DT, RF, and ADA	Hardness prediction	RF best: R^2 ≈ 0.91, RMSE≈0.99, AdaBoost close: R^2 ≈ 0.90, RMSE≈1.09 LR & DT lower: R^2 ≈ 0.84 & 0.77	Veeman *et al.*[87]
MET	PLA	Performance	CNN and RF	Process parameters–property correlation (TS and hardness)	RF accuracy: 94% (TS), 89% (hardness); CNN 88% (TS), 88% (hardness)	Butt and Mohaghegh[88]
MET	PLA	Performance	LSTM	TS prediction	R^2=89.4%	Zhang *et al.*[89]
VPP	Resin	Performance	GA+NN	Modulus and strength optimization	R^2=0.9978	Lee *et al.*[90]
MJT	Multi-material	Performance	GA	Tunable deformation and antibacterial performance	-	He *et al.*[91]
MJT	Multi-material		ANN and RSM	Shore hardness and compressive modulus optimization	ANN: MSE=0.36% (Shore A), 0.98% (E); RSM: MSE=1.3% (Shore A), 4.4% (E)	Goh *et al.*[92]

Abbreviations: ABS: Acrylonitrile butadiene styrene; ADA: Adaptive design algorithm; ANN: Artificial neural network; BO: Bayesian optimization; CNN: Convolutional neural network; DT: Decision trees; GA: Genetic algorithms; GMM: Gaussian mixture model; GPR: Gaussian process regression; KNN: K-nearest neighbors; LiR: Linear regression; LSTM: Long short-term memory; MAPE: Mean absolute percentage error; MET: Multi-exponential theory; MJT: Material jetting; ML: Machine learning; MLP: Multilayer perceptron; MSE: Mean squared error; NN: Neural network; PBF: Powder bed fusion; PCR: Principal component regression; PLA: Polylactic acid; RF: Random forest; RMSE: Root mean square error; RPU: A commercial hard polyurethane; RR: Ridge regression; RSM: Response surface methodology; SilDN: A custom soft silicone; TPU: Thermoplastic polyurethane; TS: Tensile strength; VAE: Variational autoencoder; VPP: Vat photopolymerization.

5.2.1. Material design for polymer AM

In polymer AM, material design primarily revolves around structural engineering rather than composition optimization, as modifying polymer composition is far less feasible compared to metals. To date, very few studies have employed AI for the targeted optimization of polymer feedstock composition or molecular-level properties. Unlike metals, where alloying elements can be systematically adjusted to tailor phase stability, mechanical properties, and processing behavior, polymer properties are largely dictated by their intrinsic chemical structures, molecular weight distributions, and polymerization mechanisms, making composition-based optimization significantly more constrained. In addition, synthesizing new printable polymers often requires extensive chemical modifications and rigorous processing validation, further limiting rapid material innovation. As a result, this review focuses on the AI-assisted design of mechanical metamaterials in polymer AM – an emerging direction where structural architecture, rather than chemistry, defines material performance. These metamaterials achieve properties such as auxetic behavior (negative Poisson's ratio),[93] programmable mechanical responses,[94] controlled buckling behavior,[95] shape morphing,[96] and acoustic band gap[97] through precise structural design rather than relying solely on material composition. By integrating computational modeling, ML, and multi-objective optimization, AI facilitates the design of next-generation metamaterials tailored for specific AM applications.

In polymer AM, VPP techniques are particularly well-suited for fabricating metamaterials due to their high resolution, surface quality, and processing speed. However, traditional design methodologies based on prior knowledge and intuition are increasingly inadequate for achieving next-generation metamaterial designs with optimized performance. In addition, the computational cost associated with exploring extensive lattice configurations using FEA presents a significant bottleneck, further restricting design innovation. To overcome these limitations, AI-driven approaches have been increasingly employed to automate the design process and optimize metamaterial architectures. By efficiently navigating the vast design space, AI enables the discovery of novel lattice structures with optimized properties while reducing reliance on computationally expensive simulations. This integration of AI with polymer AM facilitates the rapid development of high-performance metamaterials tailored for advanced applications. Chen *et al.*[81] developed an AI-driven computational approach for the automated discovery of mechanical metamaterials with extreme properties. Experimental validation confirms its effectiveness in discovering auxetic structures with negative Poisson's ratios, covering a broad range of elastic properties. This scalable framework extends to multiphysics metamaterials, advancing the AI-driven automated design of high-performance materials.

Similarly, Xue *et al.*[82] proposed an AI-driven optimization framework for the automated design of composite mechanical metamaterials. Their approach utilized a variational autoencoder to encode representative volume element images into a latent space, enabling efficient exploration of material distributions. Bayesian optimization (BO) was then employed to identify optimal representative volume element configurations that achieve target macroscopic elastic moduli. The optimized designs were fabricated using multi-material 3D printing and experimentally validated, demonstrating the framework's reliability in generating high-performance metamaterials.

Bessa *et al.*[84] extended AI-driven metamaterial design to brittle polymers, employing a Bayesian ML framework to develop super-compressible metamaterials. As seen in Figure 9, their approach employed sparse Gaussian processes to model uncertainty and identify recoverable structures with extreme deformation capabilities. By systematically adapting designs to different length scales and material constraints, they demonstrated the potential of AI-driven approaches in creating lightweight, tunable, and highly deformable metamaterials.

5.2.2. Performance optimization in polymer AM

Beyond metamaterial design, AI-driven approaches play a central role in optimizing process parameters and predicting material performance for polymer AM. These methods enable data-driven decision-making, significantly improving the efficiency and accuracy of mechanical performance predictions.[88,98] For example, Zhang *et al.*[89] employed a long short-term memory neural network, a DL algorithm adept at handling sequential data, to predict the tensile strength of polylactic acid components based on in-process sensor data. The model captured layer-wise temporal dependencies in FDM and achieved higher predictive accuracy than traditional ML models, underscoring the advantage of DL in time-series analysis for polymer AM.

In a generative design context, Lee *et al.*[90] applied AI-based optimization using Bézier curve manipulation and finite element simulations to design polymer lattice structures with superior mechanical performance. Their approach involved iteratively adjusting lattice beam geometries and evaluating mechanical responses, effectively shortening design cycles and outperforming human-guided design in terms of both modulus and strength.

Extending this approach to multi-material systems, He *et al.*[91] integrated GA with multi-material-inkjet 3D printing (MM-IJ3DP) and voxel-level finite element modeling. The GA served as a global search tool to explore the vast design space, enabling customizable stiffness gradients and improved biofilm resistance. As illustrated in Figure 10, their framework integrates MM-IJ3DP with FEA and GA to tailor material properties at the voxel level. Experimental validation confirmed that their approach enables the fabrication of customizable polymer composites with tunable stiffness and enhanced biofilm resistance, demonstrating the potential of AI in multifunctional material optimization.

In addition to mechanical performance, AI has been applied to enhance the biofunctional properties of polymeric AM materials.[99] In bioprinting applications, optimizing process parameters can improve biocompatibility and cell viability, while in medical implants and antimicrobial materials development, tailoring surface properties can reduce bacterial adhesion and mitigate infection risks. Magennis *et al.*[100] utilized high-throughput screening to identify polymeric materials capable of effectively resisting bacterial attachment, presenting new opportunities for biomedical AM. Figure 11 shows that their study systematically analyzed the relationship between polymer chemistry and bacterial adhesion by

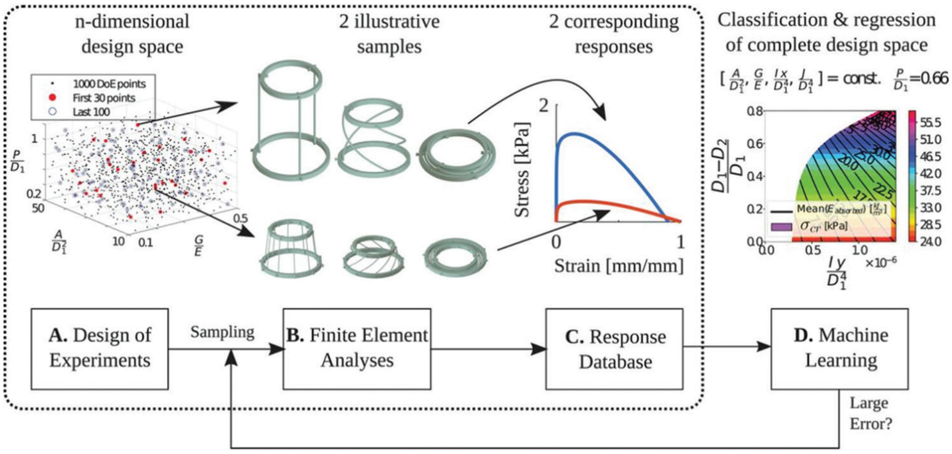

Figure 9. Bayesian machine learning framework for the design of super-compressible metamaterials in brittle polymers. Reproduced from Bessa *et al.*[84]

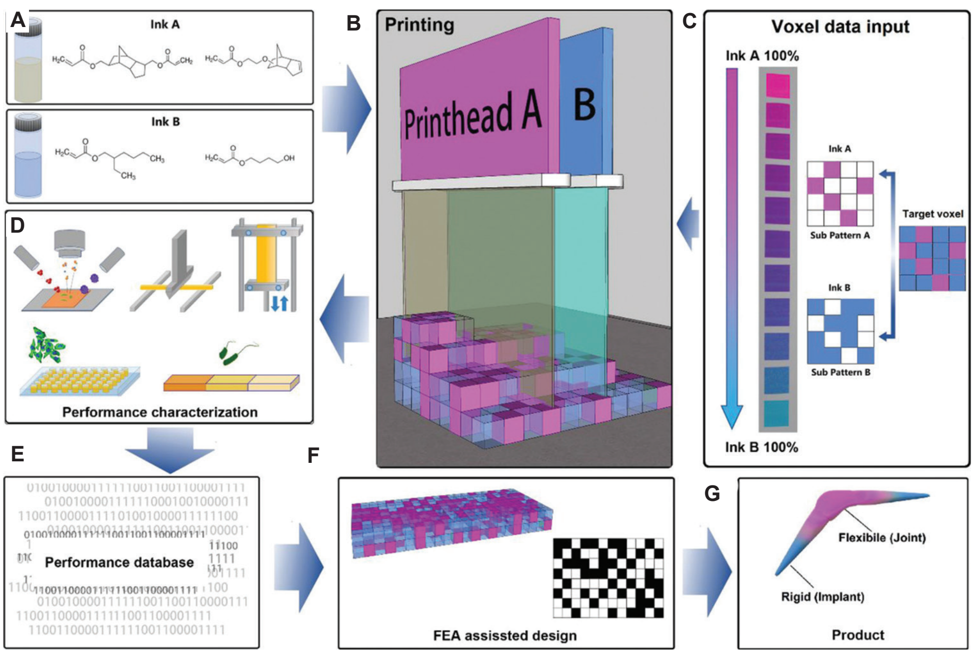

Figure 10. Artificial intelligence-driven generative design framework for multi-material 3D-printed composites. Reproduced from He *et al.*[91]
Abbreviation: FEA: Finite element analysis.

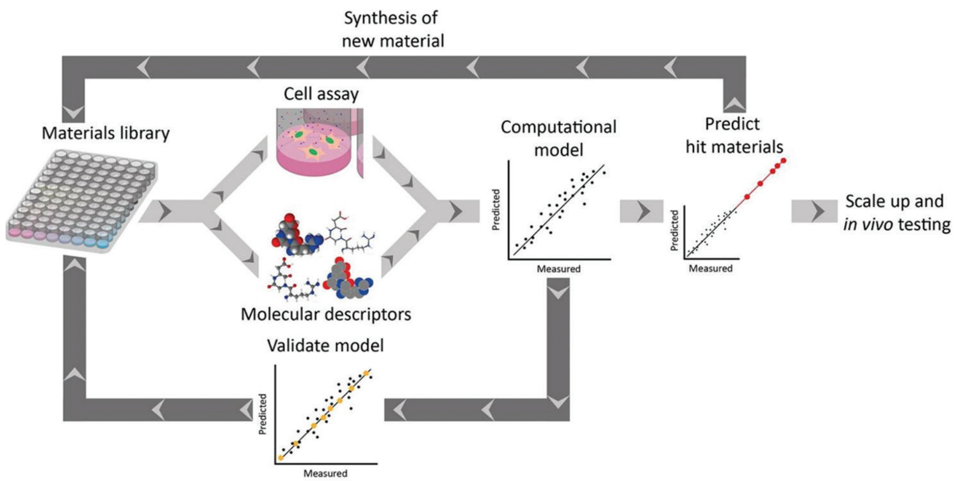

Figure 11. Process of computational modeling for the generation of novel biomaterials. Reproduced from Magennis *et al.*[100]

screening a large material library in combination with computational modeling. As a result, they identified a class of polymers with outstanding antimicrobial properties that can inhibit biofilm formation, thereby enhancing the safety of medical devices and bioprinted scaffolds. This study highlights the potential of AI and data-driven approaches in the optimization of multifunctional AM materials, demonstrating their applicability not only for mechanical enhancement but also for the improvement of biofunctional properties.

5.3. Bioink and biomaterial ink for AM

The design of bioinks and biomaterial inks is fundamental in bioprinting, as these materials form the basis for creating functional, 3D biological structures. Bioinks consist of living cells embedded within a biocompatible matrix, whereas biomaterial inks may not contain living cells but are used to construct scaffolds or structures that support cellular activities.[101] Both types of inks must be carefully formulated so that their biological and mechanical properties are compatible with bioprinting and suitable for their intended purpose after the printing process. Crafting an ideal bioink is a multi-objective problem, requiring a delicate balance of various properties, such as printability, biocompatibility, biomimicry, mechanical integrity and stability, and biodegradability.[102,103] For instance, enhancing mechanical integrity and stability often results in reduced biocompatibility, and vice versa. To discover an optimal formulation, a large number of different compositions must be tested, each representing a different trade-off between competing objectives. This is where AI becomes invaluable, significantly improving the efficiency of material search and development by helping navigate the complex multidimensional space of possible formulations.

AI approaches commonly employed in bioink and biomaterial ink design include supervised learning and reinforcement learning. In supervised learning, models are trained to predict the properties of inks in advance, allowing researchers to evaluate potential formulations quickly. Meanwhile, reinforcement learning enables models to explore the search space and identify optimal ink formulations in minimal steps, effectively learning from iterative experimentation.

On the prediction side, Qavi *et al.*[104] examined the relationship between rheological properties and printability in multi-material bioinks for extrusion-based bioprinting (EBB). Using a design of experiment approach coupled with response surface methodology, the study optimized bioink formulations containing sodium alginate, gelatin, and laponite, focusing on parameters, such as zero shear viscosity and storage modulus. By training an ANN on the obtained dataset, the relationships between the parameters were generalized, achieving a maximum mean absolute error of 6.3% in predicting the printability of the bioink formulations.

Lee *et al.*[105] addressed the challenges in designing biocompatible 3D-printable bioinks by developing an ML-based method to create viable bioinks using collagen, hyaluronic acid, and fibrin. They established a relationship between ink mechanical properties and printability, highlighting that a high elastic modulus enhances shape fidelity while extrusion remains feasible below the critical yield stress. Using multiple regression analysis, they developed a model to predict whether a composition has a high elastic modulus and low yield stress. Various bioink formulations were designed to maximize shape fidelity, leading to successful 3D constructs with viable and proliferative cells.

Xu *et al.*[106] introduced an ML framework to predict the viscosity of heterogeneous bioink compositions. Traditional models, such as the Cross model; fall short in this domain due to the non-Newtonian nature of bioinks. Their approach leveraged BO to work with sparse datasets, employing a mask technique to define feasible parameter spaces based on domain expertise. By balancing the exploration of new possibilities and exploitation of existing data, their AI-guided BO framework effectively reduced experimental workload and streamlined the building of the surrogate model for viscosity prediction.

Qiao *et al.*[107] explored the application of AI in bioink development for cryobioprinting, which integrates extrusion bioprinting and cryopreservation to enhance bioink shelf availability without using dimethyl sulfoxide due to its potential toxicity. They developed a gelatin methacryloyl (GelMA)-based bioink incorporating cryoprotective agents (CPAs) and assessed two CPA formulations, finding that ethylene glycol outperformed glycerol. Using this dataset, they established four ML models, with the ANN showing the highest predictive accuracy. This ANN model was successfully applied to predict outcomes for various CPA-based formulations, showcasing the potential of ML in the development of effective cryoprotective bioinks for cryobioprinting.

In reinforcement learning applications, Ruberu *et al.*[108] demonstrated how BO can quantitatively evaluate and optimize the printability of biomaterial inks, such as GelMA and hyaluronic acid methacrylate, by adjusting GelMA composition, ink reservoir temperature, pressure, speed, and platform temperature. They significantly reduced the number of experiments required for 3D bioprinting optimization from 10,000 to an order of 10. Hashemi *et al.*[109] also explored the development of a chitosan-gelatin-agarose biomaterial ink optimized for extrusion-based 3D bioprinting through BO. The study focused on achieving desirable mechanical properties, biocompatibility, and precise printability. The optimized ink composition (27% agarose, 53% chitosan, and 20% gelatin) showed promise for fabricating complex 3D tissue constructs. The optimized biomaterial ink exhibited sufficient viscosity for reliable printing while maintaining shape integrity in 3D structures. Biological evaluations involving bone marrow mesenchymal stem/stromal cells revealed that the ink supported favorable cell adhesion, growth, and viability.

However, a major challenge in applying AI to bioprinting is the slow collection of biologically relevant datasets, such as cell viability. A small sample size can hinder the development of robust models. To mitigate this issue, AI can be applied for fast measurement of crucial parameters using AI-driven sensors, as well as enabling rapid optimization of print parameters. For example, Huang *et al.*[110] introduced an ML-based model to predict cell numbers in bioprinted droplets by analyzing droplet velocity. Utilizing a non-destructive optical system, the study accurately detected the presence and quantity of cells in droplets. Among the evaluated models, RF regression achieved 80% accuracy for single droplet cell presence, while extra tree regression had the lowest error at 12% for cell number predictions across multiple droplets. Besides, the gel fraction of hydrogel during bioprinting can be measured with the ML or DL model through *in situ* measurement of the hydrogel's ultraviolet transmissivity.[111]

Moreover, reinforcement learning-based rapid print parameter optimization can increase sample count and efficiency. Bonatti *et al.*[112] proposed a DL-based control system to reduce the trial-and-error in EBB. The authors collected a high-resolution video dataset of various EBB parameters and trained a CNN to optimize print parameters and monitor the process in real time. This control loop halted erroneous prints to conserve resources and time while integrating the ML model with existing mathematical models, demonstrating the potential of ML to automate and ensure quality in EBB. Chen *et al.*[113] introduced an AI-assisted high-throughput printing-condition-screening system (AI-HTPCSS) to enhance the optimization of printing conditions for 3D bioprinting. This system integrated a programmable pneumatic extrusion printer with an AI-driven image-analysis algorithm to efficiently screen conditions for printing uniformly structured hydrogel scaffolds. The optimized conditions achieved through AI-HTPCSS led to scaffolds with favorable mechanical properties, improved *in vitro* biological performance, and effectiveness in enhancing diabetic wound healing *in vivo*.

The integration of AI into bioprinting has advanced bioink design by optimizing formulation properties, such as printability and biocompatibility. However, the field is still emerging, challenged by the lack of extensive datasets necessary for robust AI models. In the future, AI has the potential to revolutionize bioprinting further by enabling real-time process monitoring and adaptive control, thereby enhancing the precision and functionality of bioink development.

6. Summary

As summarized in Figure 12, this review examines how AI is transforming material development for AM, with a focus on material design and performance optimization. The integration of AI with AM processes has facilitated

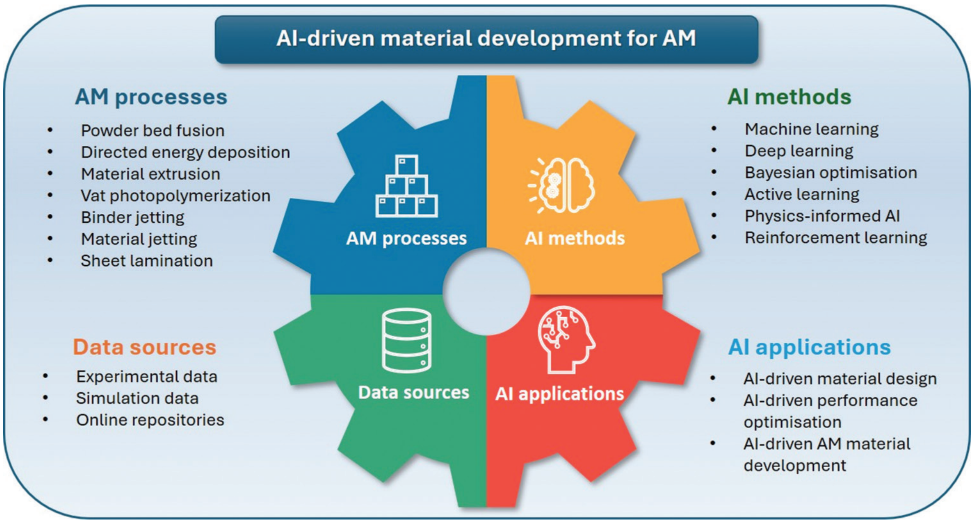

Figure 12. An overview of AI-driven material development for AM
Abbreviations: AM: Additive manufacturing; AI: Artificial intelligence.

predictive modeling, data-driven material discovery, and process optimization, significantly improving efficiency and material performance.

This review highlights the transformative role of AI in material development for AM, with particular emphasis on material design and performance optimization. Traditional trial-and-error approaches are inefficient and costly, whereas AI – particularly ML and DL – enables predictive modeling of material behavior, composition optimization, and microstructural tailoring. The integration of AI with physics-based methods, such as DFT, CALPHAD, and FEA, further enhances the accuracy and efficiency of material development workflows.

The success of AI-driven approaches depends critically on the availability of high-quality datasets. These datasets can be obtained through experimental measurements, physics-based simulations, and structured online repositories. However, most existing databases have been developed for conventional manufacturing and do not capture the process-specific features required for AM. This limitation is particularly evident under conditions involving rapid solidification and non-equilibrium phase transformations. To address this gap, there is a pressing need to construct AM-oriented datasets and apply rigorous data pre-processing procedures.

AI applications in AM material development span metals, polymers, and bioprinting. In metal AM, AI facilitates alloy design, phase prediction, and microstructure control, which helps improve printability and enhance mechanical properties. In polymer AM, AI-guided generative design supports the development of mechanical metamaterials with improved structural performance. In the context of bioprinting, AI plays a critical role in optimizing bioink formulations by balancing printability, biocompatibility, and mechanical integrity. It has also been applied to adjust extrusion parameters through reinforcement learning, thereby improving reproducibility and promoting cell viability in printed constructs. Across these domains, AI efforts are directed toward intrinsic material development, with a focus on selecting compositions, controlling phase evolution, and enhancing functional performance. This emphasis distinguishes material-centric strategies from broader manufacturing optimization. Moreover, AI improves the understanding of complex PSP relationships, which enables the design of materials with reliable and tailored properties for AM applications.

In conclusion, AI offers a paradigm shift in AM-oriented material development by accelerating the design of materials with tailored compositions and microstructures, aligned with the specific requirements of AM processes. Future progress depends on improved data availability, closer integration between AI and physical modeling, and a sustained focus on the core material properties that define performance.

7. Concluding remarks and perspectives

As discussed above, the continued advancement of AI is expected to revolutionize material development in AM by significantly enhancing predictive capabilities. By integrating AI with AM, researchers can accelerate material discovery, optimize processing conditions, and improve overall performance. Looking ahead, several key advancements are poised to shape the future of AI-driven AM materials development, as presented below.

7.1. AI-driven high-throughput material development for AM

Traditional material development for AM relies on time-consuming experimental trials and computational simulations, limiting the speed of new material discovery. AI-driven high-throughput material development offers a transformative approach by leveraging automated workflows that integrate ML, combinatorial synthesis, and rapid characterization techniques:

(i) AI-guided experimental design: ML models can predict optimal material compositions and processing conditions, reducing the need for extensive experimental iterations. By incorporating experimental data in real time, AI refines its predictions to enhance material discovery efficiency.

(ii) Automated high-throughput screening: AI has the potential to accelerate the evaluation of new alloys, polymers, and ceramics through high-throughput experimentation and combinatorial approaches, enabling the rapid assessment of microstructural stability and mechanical properties.

(iii) Inverse materials design: The prediction capacity of AI facilitates inverse materials design, allowing researchers to specify desired properties and identify compositions that meet these criteria efficiently. This approach has the potential to significantly shorten the material development lifecycle.

7.2. Integration with multiscale high-fidelity simulation with AI

While AI has demonstrated strong predictive capabilities, its full potential in AM material development requires integration with multiscale, high-fidelity simulations to improve physical accuracy and interpretability. AI can enhance and accelerate simulations in the following ways:

(i) Surrogate modeling for computational efficiency: AI-based surrogate models can approximate high-fidelity simulations (e.g., FEA, molecular dynamics, and CALPHAD) with significantly reduced computational cost, enabling rapid exploration of process–composition–microstructure relationships. For complex-shaped parts, accelerating simulations through AI should be a key research and development focus. A promising approach is to first identify defect-sensitive regions and then strategically adjust process parameters in these susceptible areas to mitigate defects.

(ii) Multiscale modeling for process optimization: AI can bridge different lengths and time scales in AM simulations, integrating macro-scale thermal simulations with microstructural evolution models to predict final part properties more accurately.

(iii) Data-driven augmentation of physics-based models: By learning from simulation outputs and experimental validation, AI improves the predictive power of physical models, correcting deviations and refining underlying assumptions. The synergy between AI and physics-based simulations will enable more accurate predictions of AM material behavior, improving process optimization and material performance forecasting.

7.3. Integration of digital twins and closed-loop design and manufacturing

The concept of digital twins – real-time virtual replicas of physical AM systems – offers new opportunities for AI-driven material design and process control. The integration of digital twins with AI enables closed-loop adaptive manufacturing, where real-time data informs continuous optimization:

(i) Real-time process monitoring and defect prediction: AI-powered digital twins integrate sensor data, *in situ* monitoring, and ML models to predict and mitigate defects such as porosity, cracking, and residual stress in AM-fabricated components.

(ii) Adaptive process control: AI-driven control systems dynamically adjust process parameters (e.g., laser power and scan speed) based on real-time feedback to optimize microstructure formation and mechanical properties.

(iii) Virtual prototyping and predictive maintenance: Digital twins enable virtual prototyping of materials and components, allowing for iterative design refinements before fabrication. In addition, predictive maintenance models help extend machine lifespan and reduce production downtime.

7.4. Active learning-driven material composition optimization for AM

One of the major challenges in AI-driven material development for AM is the scarcity of high-quality experimental data. Active learning, a branch of ML that selects the most informative data points for labeling, provides an efficient solution by minimizing experimental efforts while maximizing predictive performance:

(i) Efficient exploration of composition space: Active learning strategies guide experimental design by focusing on unexplored or high-uncertainty regions of material composition space, accelerating the discovery of optimized AM-compatible materials.

(ii) Iterative AI-experimental feedback loops: AI models dynamically update as new experimental data is acquired, refining their predictions and continuously improving the efficiency of material optimization.

(iii) BO for multi-objective design: Active learning combined with BO enables the efficient optimization of material properties while balancing trade-offs between competing factors (e.g., strength versus ductility and toughness versus printability).

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Conflict of interest

Wai Yee Yeong is an Editorial Board Member of this journal, but was not in any way involved in the editorial and peer-review process conducted for this paper, directly or indirectly. Swee Leong Sing serves as an Editorial Board Member of the journal and as the Guest Editor for the Special Issue to which this paper belongs, but he was not involved in the editorial or peer-review process for this manuscript, either directly or indirectly. Jinlong Su is a Youth Editorial Board Member of the journal and serves as a Co-Guest Editor for the same Special Issue, but similarly had no involvement in the editorial handling or peer-review of this paper. Separately, other authors declared that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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