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Artificial intelligence and machine learning in design of mechanical materials

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Artificial intelligence, especially machine learning (ML) and deep learning (DL) algorithms, is becoming an important tool in the fields of materials and mechanical engineering, attributed to its power to predict materials properties, design *de novo* materials and discover new mechanisms beyond intuitions. As the structural complexity of novel materials soars, the material design problem to optimize mechanical behaviors can involve massive design spaces that are intractable for conventional methods. Addressing this challenge, ML models trained from large material datasets that relate structure, properties and function at multiple hierarchical levels have offered new avenues for fast exploration of the design spaces. The performance of a ML-based materials design approach relies on the collection or generation of a large dataset that is properly preprocessed using the domain knowledge of materials science underlying chemical and physical concepts, and a suitable selection of the applied ML model. Recent breakthroughs in ML techniques have created vast opportunities for not only overcoming long-standing mechanics problems but also for developing unprecedented materials design strategies. In this review, we first present a brief introduction of state-of-the-art ML models, algorithms and structures. Then, we discuss the importance of data collection, generation and preprocessing. The applications in mechanical property prediction, materials design and computational methods using ML-based approaches are summarized, followed by perspectives on opportunities and open challenges in this emerging and exciting field.

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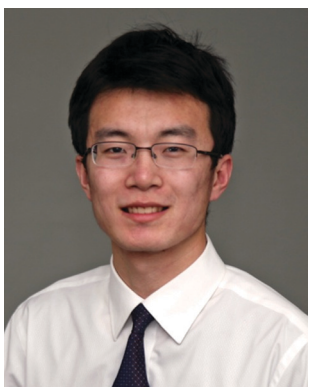

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Introduction

Materials are of significant importance to us as they are the building blocks of the tools to develop our civilization. Numerous effective methods to find new materials have been invented owing to the discovery of the intimate connection between the structure of materials and their various properties, which can be tentatively classified into mechanical, thermal, optical, electrical, chemical, nuclear, and others.[1] Among those properties, mechanical properties of materials are of particular interest owing to their intimate relationship with the integrity of structures, which ensures that the materials can consistently work as designed without mechanical failures like material degradation, cracking, buckling and delamination. Design of mechanical materials is the process of tailoring the composition and structure of materials to achieve desired or even unprecedented mechanical properties, which are of great importance to many families of advanced materials. For instance, synthetic composites can be engineered in terms of the composition of each constituent material and the structure of the composites.[2] Bio-inspired materials mimic the excellent multifunctionality including mechanical and biological properties of natural biomaterials, while difficult to design due to the complexity of hierarchical and heterogeneous structures of the mimicked biomaterials.[3–8] Another emerging category of composites that are rationally designed, called metamaterials, have attracted great interest due to their unprecedented properties compared to conventional materials, attributed to the breakthroughs in experimental techniques and computer-aided optimization tools to design complex material structures.[9,10] Architected materials, as a class of new metamaterials, have demonstrated superior mechanical properties, such as high stiffness/strength-to-weight ratios, recoverability under suppression, and damage resistance.[11–14] The complexity of compositional and topological structures of advanced materials, however, can easily lead to massive design spaces that exceed the computational limit of brute force approaches and other conventional design algorithms, implying the need for new design approaches.

Over the past a few decades, it has been found that artificial intelligence (AI), a study of computations which perceive, reason, and act like human beings, has the potential to address these challenges.[15] Specifically, the most promising one is an approach to AI called machine learning (ML), which can discover the mapping from high-throughput input data to output that is used to make decisions. In simple ML algorithms, the representation of input data is hand-designed by researchers, and each piece in the representation is referred to as a feature. Yet, it was extremely challenging to manually extract appropriate features from some sort of raw data that are easy to understand for human but difficult for machines, *i.e.*, photographs of streets where cars are supposed to be recognized, until the emerge of deep learning (DL), a specific type of ML that can not only learn the representation of the input data but also parse the representation into multiple levels—from simple features to abstract ones—attributed to complex neural network structures.[16] ML, especially DL, has achieved many exciting breakthroughs in algorithms and led to great success in computer vision, natural language processing and autonomous driving.[17] Materials and mechanics communities are aware of the great opportunities of leveraging ML as a potential new paradigm. Several general reviews of materials design using ML have been published during the past few years.[18–21] In the meantime, numerous research articles in this topic are coming out, and so do reviews of ML in specific materials or mechanics branches, involving energy materials,[22,23] glasses,[24] composites,[25] polymers,[26] bio-inspired materials,[27] additive manufacturing,[28,29] continuum materials mechanics,[30] and so on.

In this review, we focus on reviewing the growth and state of the art of research efforts on mechanical materials design using ML, and also attempt to depict a general methodology for performing ML-based mechanical materials researches. As schematically shown in Fig. 1, a typical workflow for combining ML and materials research consists of three key components: (i) a well-organized material dataset either collected from literature and

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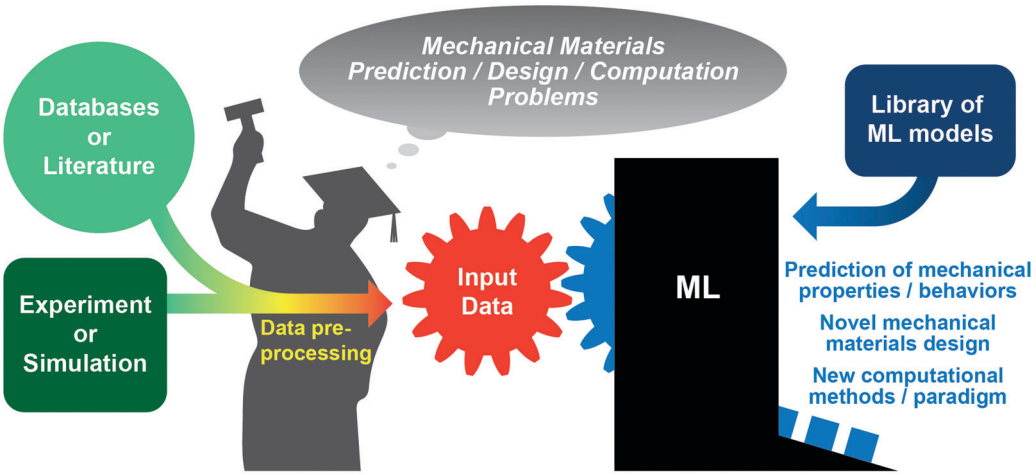

Fig. 1 Schematic of a typical workflow for design of mechanical materials using ML. With a material problem in mind, researchers encode their domain knowledge into the preprocessing of the data collected or generated from the literature, existing databases, high-throughput experiments and simulations, resulting in input data with appropriate representation that can be learned by the selected ML model, which is able to predict mechanical behaviors and/or provide novel designs of the mechanical materials of interest after training.

existing databases or generated from experiments and simulations; (ii) a ML model that is capable to learn and parse the representation for certain tasks; and (iii) a well-defined research problem of mechanical materials that has not been addressed by conventional methods, or has been solved but can be outperformed by ML-based approaches. A ML-based material research needs to glue all of these three components together, and a crucial step is the preprocessing of the raw material database into an appropriate numerical representation, also referred to as a descriptor. The preprocessed data should match the input data structure required by the selected ML model, and consist of essential material features to ensure high accuracy and training efficiency. A high-quality preprocessing requires not only expertise in mechanics and materials science, but also domain knowledge in related ML models. The former tells how to identify a challenging mechanical materials problem, acquire a database, and devise data preprocessing. The latter helps to select a suitable ML model to leverage and maximize its strength in given tasks, from prediction of mechanical behaviors of target materials, design of *de novo* mechanical materials, to development of new computational approaches.

To further discuss the foregoing methodology with the aid of present works in the literature, the paper is organized as follows. We begin with a brief summary of state-of-the-art ML models, algorithms and architectures. Readers can skip the description of the methods if they have already been familiar with them. To learn more about the methods of interest, we refer to the research articles and reviews cited in this section in which more details about the algorithms and examples are presented. Then we move on to a discussion of approaches to collect or generate datasets that are amenable to the ML models, followed by a review of existing applications of ML methods to various mechanical materials design problems. In these sections, inspiring strategies for data preparation, preprocessing, materials problem and ML model selection are highlighted. The paper is concluded with a few perspectives on the new computational paradigm that integrates mechanics and materials science with ML techniques.

A Brief summary of ML models, algorithms and structures

General ML approaches can be classified into three categories known as supervised learning, unsupervised learning and reinforcement learning (Fig. 2). Supervised learning is a task-driven approach to map inputs to outputs with data being labeled (known as the ground truth) during training, while unsupervised learning are data-driven methods trained with unlabeled data to search for undetected patterns of the given dataset. Reinforcement learning is fairly different compared to supervised learning and unsupervised learning which can be distinguished by the presence of labels. Reinforcement learning focuses on interaction between agents such as Go player with the environment such as chessboard. Both supervised learning and unsupervised learning evaluates the model's performance by minimizing a loss function or objective function. By contrast, the objective of reinforcement learning is to maximize the notion of cumulative reward. There is another category of ML approaches called semi-supervised learning. As the name implies, it lies between supervised and unsupervised learning due to the use of both labeled and unlabeled data (generally mostly unlabeled) during training. In the current field of mechanical materials designs, supervised learning approaches are most widely used as supervised tools are more accurate and mature to implement compared to the tools in other categories. Due to rapid and constant development of ML, the methods listed in the section, which cannot claim to be an exhaustive enumeration of existing ML approaches, briefly summarizes some of them that are feasible for designs of mechanical materials to the best of our knowledge.

Within this context, the simplest forms of ML without complex multilayer structures are classical ML algorithms.

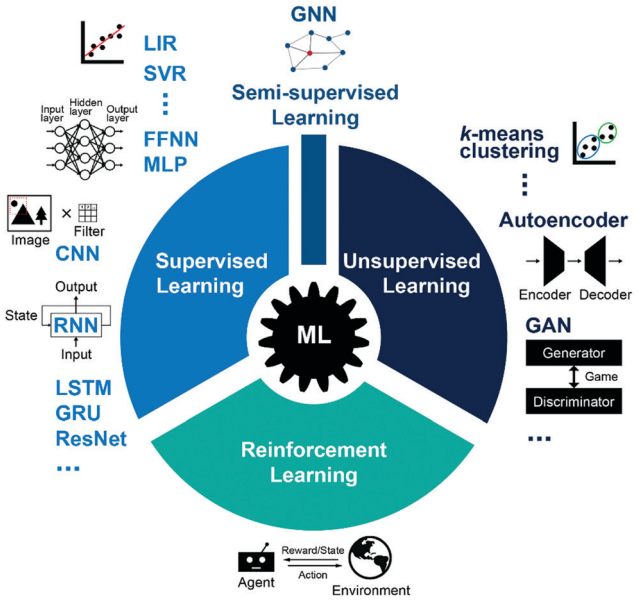

Fig. 2 A brief overview of ML approaches, including three major categories known as supervised learning, unsupervised learning and reinforcement learning. ML approaches such as linear regression (LIR), support vector regression (SVR), feedforward neural networks (FFNNs), multilayer perceptron (MLP), convolutional neural networks (CNNs) and recurrent neural networks (RNNs) are generally used for supervised learning. Typical approaches to unsupervised learning include *k*-means clustering, autoencoder and generative adversarial networks (GANs). Reinforcement learning follows a general interactive loop between the agent and the environment. The difference between supervised and unsupervised learning is determined by whether training data is labeled or unlabeled, and there is a category of tasks between them called semi-supervised learning, which combines labeled and unlabeled data (generally mostly unlabeled) during training. It is worth pointing out that some of the aforementioned ML methods are not merely limited to the tasks illustrated in this schematic. For instance, graph neural networks (GNNs) have been widely used for semi-supervised learning tasks, but they are also applicable to supervised and unsupervised learning tasks involving graph representation.

Linear regression (LIR)[31] is one of the simplest algorithms aimed to find a linear relation between the input features and continuous output. Least Absolute Shrinkage and Selection Operator (LASSO)[32] is a modification of LIR with additional absolute value penalization added to the loss function. Another reasonable extension of LIR is polynomial regression (PR)[31] which includes polynomial terms in finding linear solutions. To further support non linearity, regression algorithms such as support vector regression (SVR)[33] and random forest (RF)[34] are introduced. These nonlinear models usually handle outliers better and show higher accuracy than linear models. Apart from regression, the other major category of ML tasks is classification. Instead of predicting specific values such as housing prices, the classification algorithms classify input into predefined categories. An example of classification algorithms is logistic regression (LOR),[35] which is a classification algorithm with a loss function in logistic form despite it is named with "regression". There are many other classical ML algorithms which can handle both regression and classification problems such as decision tree (DT)[36] and gradient boosting.[37,38]

Beyond classical ML techniques, scientists have developed artificial neural networks (ANNs), loosely inspired by the interconnected neurons in human brains, for deep data mining. The original idea is derived from perceptron, a simple precursor formulation dating back to 1958.[39] By stacking multiple layers of neurons, a network structure is developed to learn nonlinear relation between input and output or delicate data distribution. As the depth of layer-by-layer networks increases, the resulting DL models offer tremendous impacts in computer science and various related interdisciplinary areas.

Feedforward neural networks (FFNNs) or multilayer perceptron (MLP)[40,41] are probably the simplest and quintessential DL models. As the names indicate, the information passes through the network in a unidirectional manner for FFNNs. More specifically, each layer which consists of multiple neurons computes the output to the next layer based on the input from the previous layer. The weights or trainable parameters used for calculation for each neuron are optimized to minimize the loss function. In order to approach the minimum of the loss function during the training process, back propagation (BP), a widely used technique in ANNs training, is implemented together with gradient descent (GD) algorithm.[42] BP functions as similar as calculating derivatives and GD algorithms determine the direction to jump down to the minimum. The process iterates until the loss function is close to its minimum.

Besides general FFNNs, two types of DL architectures are gaining vast attention due to their applications in computer vision and natural language processing (NLP), known as convolutional neural networks and recurrent neural networks.

Convolutional neural networks (CNNs) were first introduced in 1980,[43] and reformulated in 1999.[44] CNNs are image-based DL architecture by calculating mathematical operation "convolution" to extract features of images. Convolution preserves the spatial relationship between pixels and is calculated by multiplying the image matrix with the filter matrix. Filters contain trainable weights which are optimized during training for feature extraction. With different filters, separate operations such as edge detection can be performed to one image. By stacking the convolutional layers, simple features will be gradually assembled to intact and complicated ones.[45] The CNNs are applied to and show exciting performances in face recognition, images classification and object detection.[40] In materials design problems, with the capacity of capturing features at different hierarchical levels, CNNs are well suited to describe the properties of materials (which innately have hierarchical levels), especially biomaterials. These hierarchical features are not just found in materials, but in many other representations of matter, sound and language, and hence universal to the description of key societal systems.[46,47]

Recurrent neural networks (RNNs) also gain popularity due to their capability of dealing with sequential data. In CNNs, inputs and outputs are supposed to be independent of each other, which might not be suitable for some tasks that emphasize the sequence of the data. For instance, given an incomplete sentence, it would be difficult to predict the next word if the sequential structure of the sentence is omitted. Instead, RNNs act on the sequential data with the output being depended on the previous and later sequence and utilize "memories" in determining output of each layer or state. For RNNs with large depth, the gradient calculated by BP easily

vanishes or explodes.[48,49] To address this issue, plenty of mechanisms including Long short-term memory (LSTM),[50] Gated recurrent unit (GRU),[51] ResNet[52] and Attention[53,54] have been developed, increasing the impact of RNNs in NLP tasks such as language translation and speech processing. RNNs also shed light on scientific problems such as protein folding and *de novo* protein design.[55–57]

Generative models have been established to generate new data points based on the distribution of existing data. An intriguing and successful category of architectures among them are generative adversarial networks (GANs),[58] which consist of two neural networks, the generator and the discriminator. The generator proposes new data instances and the discriminator compares the generated data with the real data. These two components contest with each other during the training as the generator aims to ''fool'' the discriminator by producing more genuine images while the discriminator attempts to distinguish real images from false images as accurately as possible. GANs reach convergence when the generator and the discriminator are at Nash equilibrium. The process of balancing the performances of the generator and the discriminator is somewhat similar to equilibrating a physical system with both attractive and repulsive forces which indicates that GANs can potentially shed light on describing physical phenomena. Furthermore, with the objective of generating fake data with restricted conditions or characteristics, a subtype of GANs named conditional GANs (cGANs)[59] have been developed which include labels as a control variable. One of the applications of cGANs is image-to-image translation[60,61] in which an image is used as the constrain of the generator. Unlike GANs, variational autoencoder (VAE)[62] is another type of generative models that uses one neural network which first encodes the input data into an inexplainable code named as latent code and then decodes the latent code to reconstruct the output.

ML methods can also be used to evaluate and improve the performance of other applied ML models. Bayesian learning (BL)[40] is an approach used for parameter estimation and probability comparison to evaluate a given algorithm. Gaussian process regression (GPR)[63] is a nonparametric approach which can provide uncertainty measurements of predictions and build reduced-order models based on Bayesian learning. These approaches are potentially useful for mechanical materials designs problems as they are suitable for relatively small datasets and are working well without prior knowledge of model forms. Moreover, active learning is a learning algorithm that interactively inquires the user and selects data to be labeled.[64] Training data would be augmented in an active learning loop with post-hoc experiments or simulations. For further discussion on the application of active learning in materials science, we refer to a recent review paper.[65]

Reinforcement learning (RL) is an area of ML in which the agent takes action based on the variation of the environment to maximum long-term gains.[66] The training process is aiming at finding a balance between exploration (of uncharted territory) and exploitation (of current knowledge).[66] From 2014 to 2017, the presence of AlphaGo,[67] a RL-based AI was able to beat top-notch Go players, showing the power of RL and its potential applications to materials problems such as interactive materials design.

Graph neural networks (GNNs), unlike standard neural networks operating on Euclidean data, operate on graphs that have non-Euclidean data structures consisting of nodes connected by edges without natural orders.[68] Recent breakthroughs in GNNs, such as graph convolutional networks (GCNs),[69] have demonstrated the capability of GNNs to learn graph embeddings through message passing between the nodes and its outstanding performance on semi-supervised classification tasks, which are potentially applicable to many materials and mechanics problems that inherently consist of graph structures.

Popular ML models and algorithms used in the design of mechanical materials, along with example applications, are tabulated in Table 1.

Data collection, generation and preprocessing

If ML models are the engines to tackle various tasks, then data is the fuel to power the models. Sufficient amount of data is a prerequisite to make the models work, and high-quality data enable the models to run efficiently. Nevertheless, there arise several vital and difficult questions: how much data is sufficient? How to obtain those data? What is the quality of the input data? And how to improve it? These questions are crucial for the ML-based design of mechanical materials since the data relate the mechanics problems of interest to the applied ML models. Researchers can either collect data from the literature or existing databases, or generate their own databases *via* high-throughput experiments or simulations (Fig. 1). Feeding the raw data into the ML model is usually accompanied with the following issue: when the data is either too easy or too hard to be obtained, it would be unnecessary or difficult to implement ML-based methods for solving the problem. For instance, there is no need to use ML if the existing method can travel through the entire design space at an acceptable cost, and a more common scenario is that the obtained datasets only cover a small portion of the design space. It is also possible that the collected databases of images or texts are understandable for human but uninterpretable for machines. In those cases, the raw data are, in general, required to be preprocessed before fed into the ML model, emphasizing the importance of leveraging the domain knowledge of the researchers to obtain representative data and perform data preprocessing in a proper manner for better results from the ML model. In this section, we briefly review and discuss some methods for data collection, generation and preprocessing in the literature that might shed light on the study of mechanical materials design problems using ML, including several pioneering approaches developed for data-driven computational mechanics,[70–73] and data-driven frameworks of materials analysis and design.[74–81]

Data collection from existing databases or literature

The advent of high-throughput computational materials design leads to the construction of many materials databases,[82] such as AFLOW,[83] Materials Project (MP),[84] MATDAT,[85] MatWeb,[86]

Table 1 Popular ML methods in design of mechanical materials

ML method	Characteristics	Example applications in mechanical materials design
Linear regression; polynomial regression	Model the linear or polynomial relationship between input and output variables	Modulus[112] or strength[123] prediction
Support vector machine; SVR	Separate high-dimensional data space with one or a set of hyperplanes	Strength[123] or hardness[125] prediction; structural topology optimization[159]
Random forest	Construct multiple decision trees for classification or prediction	Modulus[112] or toughness[130] prediction
Feedforward neural network (FFNN); MLP	Connect nodes (neurons) with information flowing in one direction	Prediction of modulus,[97,112] strength,[93] toughness[130] or hardness;[97] prediction of hyperelastic or plastic behaviors;[143,145] identification of collision load conditions;[147] design of spinodoid metamaterials[163]
CNNs	Capture features at different hierarchical levels by calculating convolutions; operate on pixel-based or voxel-based data	Prediction of strain fields[104,105] or elastic properties[102,103] of high-contrast composites, modulus of unidirectional composites,[136] stress fields in cantilevered structures,[137] or yield strength of additive-manufactured metals;[121] prediction of fatigue crack propagation in polycrystalline alloys;[140] prediction of crystal plasticity;[120] design of tessellate composites;[107–109] design of stretchable graphene kirigami;[155] structural topology optimization[156–158]
Recurrent neural network (RNN); LSTM; GRU	Connect nodes (neurons) forming a directed graph with history information stored in hidden states; operate on sequential data	Prediction of fracture patterns in crystalline solids;[114] prediction of plastic behaviors in heterogeneous materials;[142,144] multi-scale modeling of porous media[173]
Generative adversarial networks (GANs)	Train two opponent neural networks to generate and discriminate separately until the two networks reach equilibrium; generate new data according to the distribution of training set	Prediction of modulus distribution by solving inverse elasticity problems;[138] prediction of strain or stress fields in composites;[139] composite design;[164] structural topology optimization;[165–167] architected materials design[115]
Gaussian process regression (GPR); Bayesian learning	Treat parameters as random variables and calculate the probability distribution of these variables; quantify the uncertainty of model predictions	Modulus[122] or strength[123,124] prediction; design of supercompressible and recoverable metamaterials[110]
Active learning	Interacts with a user on the fly for labeling new data; augment training data with post-hoc experiments or simulations	Strength prediction[124]
Genetic or evolutionary algorithms	Mimic evolutionary rules for optimizing objective function	Hardness prediction;[126] designs of active materials;[160,161] design of modular metamaterials[162]
Reinforcement learning	Maximize cumulative awards with agents reacting to the environments.	Deriving microstructure-based traction-separation laws[174]
Graph neural networks (GNNs)	Operate on non-Euclidean data structures; applicable tasks include link prediction, node classification and graph classification	Hardness prediction;[127] architected materials design[168]

MatMatch,[87] MakeItForm,[88] and MatNavi.[89] These databases consist of enormous materials properties obtained from experimental measurements and first-principles calculations, including mechanical properties like elastic constants, tensile/flexural/shear/fatigue strengths, fracture toughness, hardness, and so on. Detailed mechanical features of these databases are listed in Table 2. According to the mechanical problems of interest, sub-datasets of specific properties or material classes can be filtered and collected effectively through the online platforms of those databases. For instance, mechanical properties of inorganic compounds from the MP database have been systematically explored.[90] In a separate study, more than one hundred vanadium oxide materials along with various unique compositions have been found in the MP database.[91] In order to train DL models, this dataset has been significantly enlarged *via* a virtual substitution of existing binary materials. As an inspiring example, Raccuglia *et al.* have leveraged the unreported entries about failed experiments from their archived laboratory notebooks to build a database for use in training and testing the applied ML model.[92]

Labeled datasets can be obtained from surveying the literature as well, such as datasets of copper alloys with different tensile strengths and electrical conductivities,[93] ABO_3 compounds,[94] high-temperature ferroelectric perovskites,[95] and single-molecule magnets.[96] In addition, a glass dataset of experimental data was

Table 2 High-throughput materials databases with mechanical features

Database name	Material categories	Mechanical features	URL
AFLOW[83]	Alloys; inorganic compounds	Elastic properties	http://www.aflowlib.org/
Materials Project (MP)[84]	Inorganic compounds; nanoporous materials	Elastic properties	https://materialsproject.org/
MATDAT[85]	Steels; aluminum and titanium alloys; weld metals; *etc.*	Static properties; nonlinear stress-strain behaviors; cyclic stress–strain behaviors; fatigue behaviors	https://www.matdat.com
MatWeb[86]	Polymers; metals; ceramics; semiconductors; fibers; *etc.*	Elastic properties; strength; toughness; hardness; *etc.*	http://www.matweb.com
MatMatch[87]	Metals; composites; ceramics; polymers; glasses; *etc.*	Elastic properties; strength; toughness; hardness; *etc.*	https://matmatch.com
MakeItForm[88]	Metals; polymers; ceramics	Elastic properties; strength; toughness; hardness; *etc.*	https://www.makeitfrom.com
NIMS materials database (MatNavi)[89]	Polymers; inorganic materials; metals	Elastic properties; strength; hardness; *etc.*	https://mits.nims.go.jp/en/

collected from both literature and existing databases.[97] The size of the collected dataset relies heavily on the amount of accumulated literatures in the corresponding field. Relatively small datasets with tens to hundreds data points are acceptable for optimization approaches if equipped with an active learning loop.[95,98]

Furthermore, text processing techniques can be utilized to replace manual labor in the extraction of features from research articles. With NLP techniques adopted, an automated workflow of article retrieval, text extraction and database construction was developed. to build a dataset of synthesis parameters across 30 different oxide systems, which is autonomously compiled and tabulated by training the text processing approach using over 640 000 materials synthesis journal articles.[99] The materials synthesis databases obtained from this approach enable a broader applications of ML methods than before, such as the prediction of materials synthesis conditions[100] and candidate precursors for target materials.[101]

Data generation

When performing high-throughput experiments or simulations, researchers have more freedom to design the features and control the size and distribution of the datasets to be generated. Nevertheless, a major challenge is to balance the expense of data generation and the resulting performance of the applied ML model. Existing works in the literature have shown that leveraging domain knowledge in materials science, solid mechanics and other related fields results in datasets that are more representative of the design spaces and thus display better results from the applied models.

Computational methods can be used to simulate materials of interest and relate the mechanical properties to the representative structures of the materials at different scales, from continuum to atomistic levels. For example, finite element method (FEM) was implemented to generate datasets of three-dimensional (3-D) microstructures of high-contrast composites,[102–106] two-dimensional (2-D) tessellate composites,[107–109] and metamaterials.[110] Yang *et al.* created a dataset of synthetic microstructure images of materials with various compositional and dispersive patterns using Gaussian random field (GRF) method.[111] High-throughput molecular dynamics (MD) can be utilized as a design space sampling method for the atomistic structures and behaviors of materials like silicate glasses,[112] metal–organic frameworks (MOFs),[113] as well as brittle materials with different crystal orientations.[114]

A framework for data-driven analysis of materials has been built to avoid unacceptable computational expense of data generation from high-fidelity analyses, such as FEM simulations involving plasticity and damage, and reduced order methods were utilized to generate large databases suitable for ML.[77,78,81] It is also possible to reduce the scale of design spaces by considering the symmetries in the materials problems to be investigated. The design spaces of 2-D tessellate composites under symmetric loadings can be truncated by half,[107–109] and the generated topologies of architected materials were classified into 17 datasets according to the crystallographic symmetry groups in 2-D space.[115]

Benchmark databases, such as MNIST,[116] are particularly useful for comparing the accuracy and efficiency of various ML techniques on specific tasks. Recently, a benchmark dataset named Mechanical MNIST was constructed by converting the MNIST bitmap images into heterogeneous blocks of materials.[117] This dataset, labeled by different forms of mechanical responses calculated from FEM simulations, can be used to evaluate the performance of metamodels of heterogeneous materials under large deformation.

Performing experiments to create sufficient large datasets for training DL models is currently difficult due to the extremely high cost. However, high-throughput experiments are applicable to the validation of trained ML models,[118] and relatively small training sets can be augmented *via* post-hoc experiments in an active learning loop.[95,98] Recently, an autonomous research system has been built to enable not only automated experimentation but also the selection of subsequent experiments under a framework of Bayesian optimization, which can be utilized to mechanical materials design problems such as optimization of additive manufacturing structures.[119]

Data preprocessing

ML models expect certain data structures (*i.e.*, images, texts, graphs) as input and thus the datasets need to be preprocessed before fed into the applied model. During preprocessing, data

augmentation techniques can be implemented to enlarge the datasets, and irrelevant data points that would deteriorate the performance of the model should be removed.

In a recent work on the prediction of fracture patterns in brittle materials, the discrete atoms in a triangular lattice, which is adopted from the MD simulations to generate the datasets of crack patterns, were mapped into ordered pixels in an image that can not only be treated as input to the first convolutional layer of the applied LSTM model but also eliminate the irrelevant information in the atomic structure other than the spatial features of the crack.[114] In another example, least angle regression (LARS) was utilized as a feature selection algorithm for a large glass dataset taken from the literature and online databases.[97] Image processing techniques, such as rescaling and cropping, were utilized to augment the initial dataset that might be insufficiently large to train a DL model.[120] It has been demonstrated that less efforts on preprocessing are required to design features for DL than conventional ML methods due to the ability of the DL models to parse the representation from simple to abstract features through the training process.[121] The techniques used to develop data-driven solvers might also inspire efficient methods to process sparse and noisy data of materials responses.[70,71]

Applications

Prediction of mechanical behaviors

The ML models, trained on the datasets containing materials information, are supposed to give fast and accurate predictions of target mechanical properties or behaviors, or to discover compositions or structures that outperform the training data in the design space.

Materials with complex and disordered microstructures, such as glasses and alloys, typically have large databases obtained from experiments or simulations focusing on composition-property relationships. Thus, the selected features like concentrations of components are usually arranged as feature vectors, and ML methods good at processing input vectors are particularly suitable for the property prediction tasks of these materials. For instance, different ML algorithms (PR, LASSO, RF and MLP) were adopted to predict the Young's modulus of silicate glasses.[112] Among those methods, MLP gives the highest accuracy, and the LASSO algorithm offers a slightly lower accuracy but higher simplicity and interpretability of the model. It is subsequently shown that using GPR instead of neural networks can avoid overfitting for a sparse dataset.[122] Recently, a large dataset obtained from the literature and glass datasets was preprocessed to train deep FFNNs that allow the design of eight essential properties of oxide glasses, including Young's modulus, shear modulus and hardness.[97] Wang *et al.* developed a design system based on neural networks for copper alloys that can rapidly screen the composition design space and provide the compositional design of new copper alloys with a target ultimate tensile strength and electrical conductivity.[93] To discover strong and conductive copper alloys, Zhao *et al.* recently reported a systematic study of the selection of ML models (LIR, SVR, regression tree and GPR), dimensionality reduction techniques (principal component analysis, correlation-based and genetic algorithm) and additional features.[123] For gradient nanostructured metals, Gaussian process based active learning surrogate models were developed to study the structural gradient effects on strength and deformation mechanisms.[124] Furthermore, new superhard materials were proposed with the aid of ML techniques such as SVR,[125] evolutionary algorithms,[126] and GNNs.[127] In a study by Wen *et al.*, high entropy alloys predicted by the applied ML models were synthesized, showing higher hardness values than any other sample in the training dataset.[128] ML models can also be trained to capture the relationship between salient structural features and mechanical properties. For example, deep neural networks that were trained to learn the relationship between the geometric patterns and mechanical responses of non-uniform cellular materials are capable of solving both forward and inverse problems.[129] Liu *et al.* have achieved the fracture toughness prediction of polycrystalline silicon specimens using two different ML algorithms, RFs and FFNNs.[130] In a recent study, the strength and toughness of spider webs were predicted by using a neural network trained with fiber lengths and orientations, as well as web connectivity and density.[131]

ML-based prediction of mechanical properties can also be achieved using atomistic descriptors. For example, local properties (bond length, angle and dihedrals), global properties (density or ring sizes distribution) and porosity-related properties were fed as entries into a gradient boosting regressor to predict mechanical properties of zeolite frameworks.[132,133] Given the system temperature, strain rate, vacancy defect and chirality, mechanical properties of single-layer graphene were predicted using different ML algorithms (stochastic gradient descent, *k*-nearest neighbors, SVR, DT, ANN).[134] In a separate work by Moghadam *et al.*, the relationship between the structure and mechanical stability of thousands of MOF materials has been established to predict the bulk modulus of MOF materials using an ANN that inputs structural or topological descriptors.[113]

For materials that can be represented as tessellated spatial grids of multi-phase voxels, CNNs are advantageous over conventional ML methods in learning embeddings at different length scales ranging from voxels to representative volume elements (RVEs). The elastic deformation fields and effective elastic properties of high-contrast two-phase composites were predicted using 3-D CNN and datasets of 3-D volume elements with different microstructures (Fig. 3).[102–105] Convolutional networks with different architectures were used to predict the mechanical properties of polymer nanocomposites based on microstructure images,[135] thermo and mechanical properties of unidirectional composites,[136] and stress fields in cantilevered structures.[137] In particular, Herriott and Spear implemented two conventional ML methods (Ridge regression and gradient boosting) and a CNN model to predict the effective yield strength of additive-manufactured metals.[121] When 3D images of the microstructures represented by crystal orientation are input to the CNN model, it outperforms the other two methods fed with microstructural features, demonstrating the strengths of CNN in learning higher-level features directly from image data and reducing the efforts on preprocessing and feature extraction.

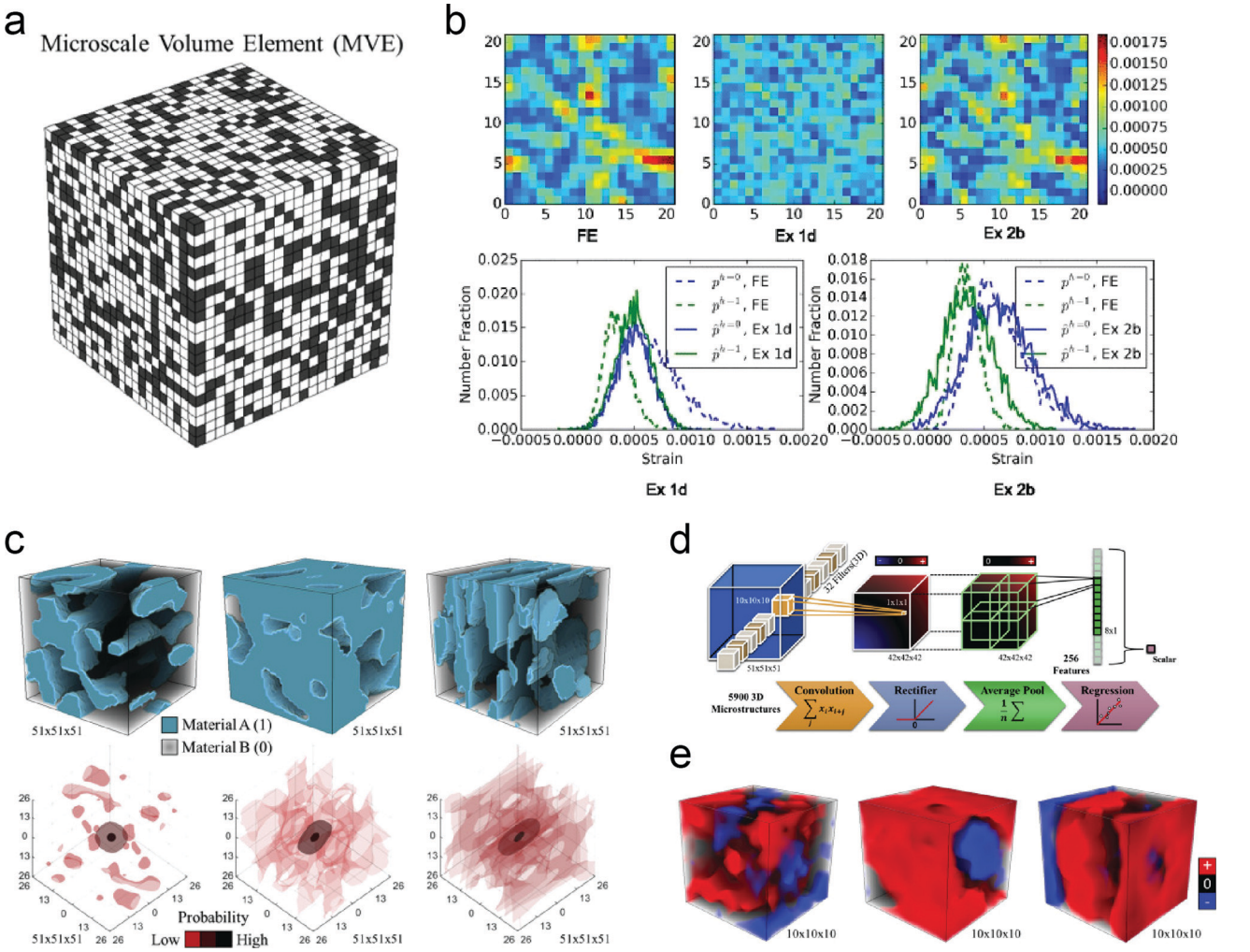

Fig. 3 Predicting elastic behaviors of high-contrast composites using convolutional neural network (CNN). (a) An example microscale volume element, and (b) a comparison of strain field prediction from FEM and statistical models. (Licensed under CC-BY).[104] (c) The compositional structures (top) and spatial statistics (bottom) of three example generated microstructure volume elements, (d) a schematic of the applied 3-D CNN architecture, and (e) a selection of three learned filters that help to distinguish microstructures similar to the three examples shown in (c), respectively (Reproduced with permission.[103] Copyright 2017 Elsevier).

The capability of generative models to deal with image-to-image translation tasks can be harnessed to achieve fast conversion between material distribution and mechanical fields. Ni and Gao developed a cGAN model to address the inverse elasticity problem of calculating elastic modulus distribution from observed displacement or strain fields in inclusion systems, mimicking an application scenario for real-time elastography and high-throughput non-destructive evaluation techniques.[138] Recently, Yang *et al.* introduced a deep learning approach which predicts complex strain or stress fields of hierarchical composites directly from geometric information.[139] Image-to-image translation using GANs has been implemented to investigate mechanical systems and exhibited astonishing performances in reproducing mechanical fields, extracting secondary information and extending to various loading conditions, component shapes and hierarchies. This framework could be further applicable to fast prediction of other physical fields with geometric information in image-based representation.

Mechanical problems involving nonlinearities such as plasticity, fracture and dynamic impact are known to be difficult and computationally expensive for conventional numerical simulation schemes. ML-based approaches have created new opportunities for addressing these long-standing problems.

For fracture problems, Pierson *et al.* developed a CNN-based methodology to predict the microstructure-sensitive propagation of a 3-D fatigue crack in a polycrystalline alloy based on the past crack surface.[140] Guilleminot and Dolbow reported a data-driven framework that can generate new crack patterns in random heterogeneous microstructures through the combination of a manifold learning approach and a crack path reconstruction procedure.[141] Moreover, Hsu *et al.* presented a ML-based approach combining convolutional layers and LSTM for predicting fracture patterns in crystalline solids based on atomistic molecular simulations (Fig. 4a).[114] The proposed approach not only captures complex fracture processes but also

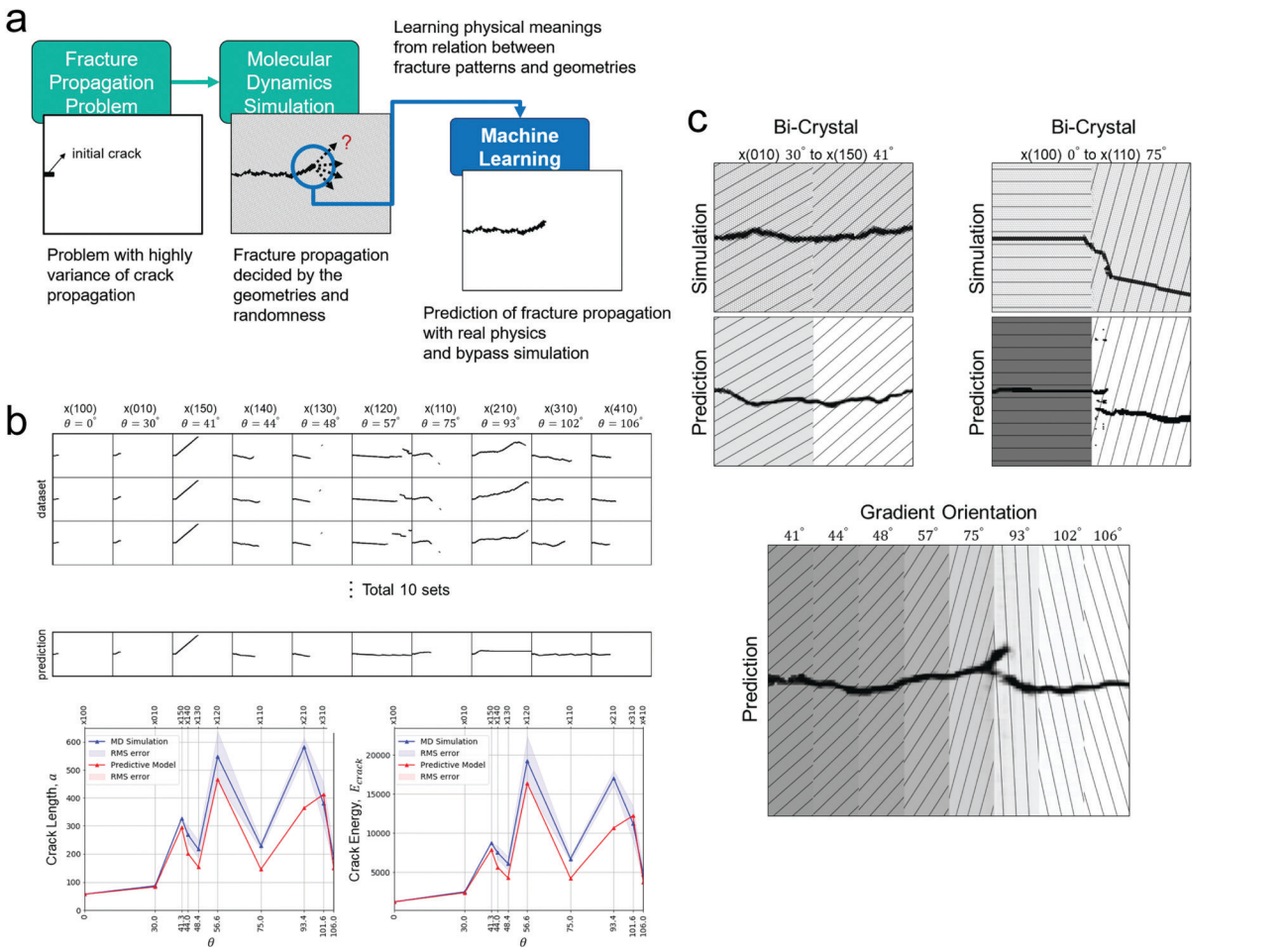

Fig. 4 Predicting dynamical fracture using a deep learning approach, dependent on microstructural details. (a) Workflow of fracture patterns prediction. (b) Comparison of crack path, length and energy release between molecular simulations and the ML approach. (c) Prediction of crack patterns in bicrystalline and gradient materials (Reproduced with permission.[114] Copyright 2020 Elsevier).

shows good agreement regarding fracture toughness and crack length (Fig. 4b). The work further examined the crack propagation in more complicated crystal structures including bicrystalline materials and graded microstructures (Fig. 4c). The strong predictive power of their approach can be potentially applied to design materials with enhanced crack resistance.

For nonlinear deformation problems, Mozaffar *et al.* recently established a data-driven framework consisting of RNNs to learn history-dependent behaviors of heterogeneous RVEs loaded along different deformation paths, and it has enabled the prediction of plasticity-constitutive laws in an efficient and accurate manner without adopting the widely-used assumptions in existing plasticity theories (Fig. 5).[142] Huang *et al.* developed a hyperelastic model using FFNNs and a plasticity framework *via* a combination of FFNNs and Proper Orthogonal Decomposition (POD).[143] Yang *et al.* trained a deep residual network that can predict crystal plasticity using high-throughput discrete dislocation simulations.[120] Wu *et al.* designed a RNN based on GRU to predict the stress–strain evolutions of elasto-plastic composite RVEs subjected to random loading paths.[144] Yang *et al.* utilized ANNs to construct constitutive laws for isotropic hardening elastoplastic materials with complex microstructures.[145] In a study by Zhou *et al.*, a discrete dislocation dynamics model of straight dislocations on two parallel slip planes was self-consistently transformed into a continuum model *via* the integration of asymptotic analysis and ML methods.[146] Chen *et al.* utilized DL models to find the inverse solution to collision load conditions with the post-collision plastic deformation of shell structures given.[147] Stern *et al.* reported a framework for supervised learning in thin creased sheets which can not only accurately classify the patterns of training forces but also generalize to unseen test force patterns, demonstrating how learning can be achieved from plasticity and nonlinearities in materials.[148] In order to solve both forward and inverse indentation problems, many efforts have been made using neural networks.[149–153] Recently, Lu *et al.* demonstrated a general framework for extracting elastoplastic properties of materials from instrumented indentation results with significantly elevated accuracy and training efficiency, which have been furtherly improved by considering known physical and scaling laws and by utilizing transfer learning techniques when additional new experimental data are available.[154]

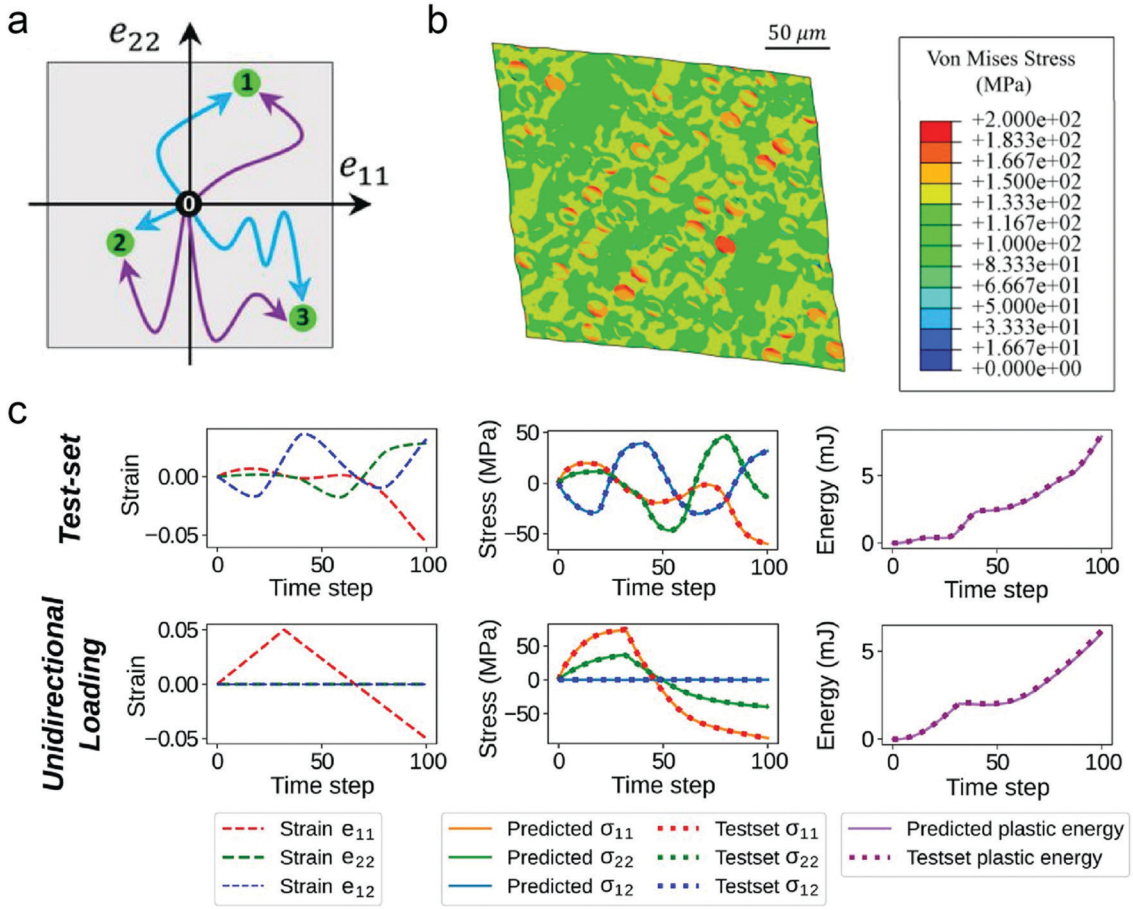

Fig. 5 Learning history-dependent plasticity using recurrent neural networks. (a) Schematic of sampling temporally deformation paths. (b) A deformed heterogeneous representative volume element (RVE) with distributed circular fillers in the generated database. (c) Comparison of the results predicted by recurrent neural networks and calculated from FEM analyses for two different RVEs under different loading conditions (Licensed under CC-BY).[142]

Topological design

Designing topological structures of multi-phase materials such as composites or architected materials is intractable in some aspects for conventional optimization methods due to the dauntingly large design spaces, while ML-based models have the capability to explore the design spaces more efficiently and to find unprecedented designs with better performance than the structures in training sets.

2-D structures of materials can be represented as pixel images, fed as input to image processing models like CNNs and GANs. These models can significantly enlarge the design spaces to be explored for the optimal design, and the design process can be furtherly accelerated through the integration of appropriate optimization algorithms in the workflow. For instance, Gu *et al.* used CNN to design tessellate composites with optimized strength and fracture toughness (Fig. 6a–d).[107,108] CNN was applied to extract local patterns of the composite around the crack tip in the framework. In these problems, the scale of the design space increases exponentially with the number of grid elements in the composites, and finding the optimal design can be easily intractable for brute-force approaches by elevating the grid resolution. In order to address this issue, Yu *et al.* integrated the CNN model with a genetic algorithm to accelerate the search process using the ML prediction as the fitness function for the optimization algorithm (Fig. 6e and f).[109] In a study by Hanakata *et al.*, a CNN-based search algorithm was developed to find optimal arrangements of kirigami cuts in graphenes to maximize stretchability.[155]

Encoder and decoder frameworks based on convolutional layers can be employed to accelerate the process of topology optimization of mechanical structures.[156–158] Since the models were trained with the structures that have already been optimized by standard optimization methods, direct evaluation of mechanical properties (*e.g.*, compliance) in loss functions can be avoided. As a trade-off, designs predicted by ML models may have mechanical incompatibility such as structural discontinuity, but these issues can be refined by connecting a cGAN model to the trained encoder and decoder network.[156] Different from a pixel-based representation, a structural topology optimization method has been achieved through the movement of morphable components as basic building blocks, and both SVR and the *k*-nearest neighbors algorithm were adopted to extract the mapping between the external load and design parameters.[159] Even though this approach shrinks the design space, it can

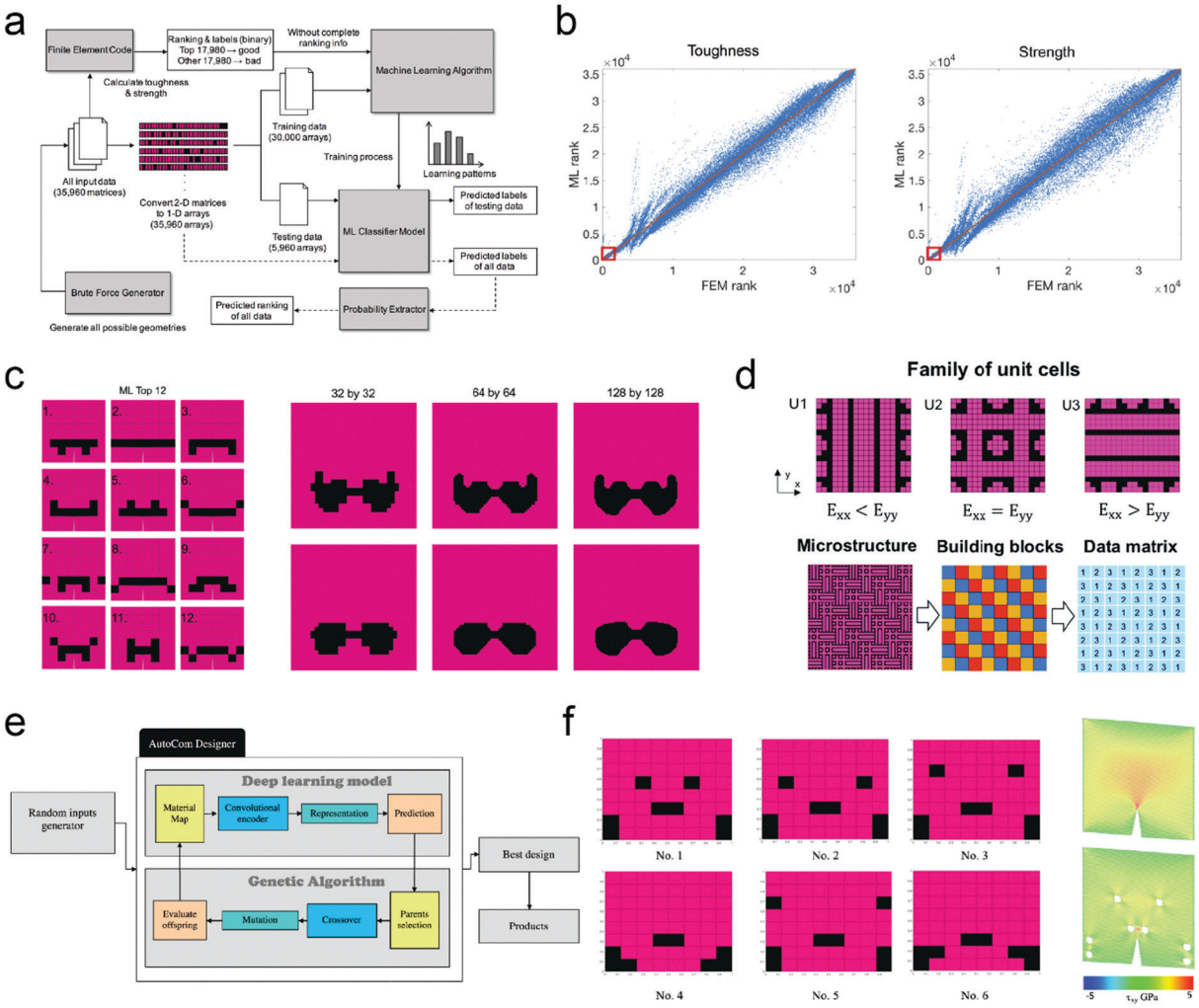

Fig. 6 ML-based tessellate composites design for optimal strength and fracture toughness. (a) Workflow of the ML approach for the prediction of mechanical properties of composites. (b) Ranking comparison between the results from the ML approach and FEM simulations. (c) Optimal designs regarding strength and toughness in mode I test at various resolutions (Reproduced with permission.[107] Copyright 2017 Elsevier). (d) Extended implementation to composites consisting of anisotropic building blocks (Licensed under CC-BY).[108] (e) Framework embedded with genetic algorithm to accelerate the design process and (f) optimal designs in mode II test validated by MD simulations (Reproduced with permission.[109] Copyright 2019 IOP Publishing Ltd).

avoid mesh dependency and model complexity issues induced by preprocessing structures into pixel images.

Topological design approaches using other ML techniques have also been widely reported in the literature. For example, structural designs of active composite beams and hard-magnetic soft active materials with target deflected shapes were obtained using evolutionary algorithms.[160,161] Recently, Wu *et al.* reported an approach to design modular metamaterials using genetic algorithm and neural networks.[162] They applied the method to the design problems of phononic metamaterials and optimization problems of interconnect for stretchable electronics. Kumar *et al.* built an inverse design framework of spinodoid metamaterials using deep neural networks that can provide optimal topologies for desired properties.[163]

Leveraging the strengths of advanced ML techniques usually offers new pathways for the design of mechanical materials. Bayesian machine learning is a powerful approach for handling noisy data and can quantify the uncertainty of model predictions, which are particularly useful for design of metamaterials that are often sensitive to manufacturing imperfections. Bessa *et al.* demonstrated that data-driven designs of supercompressible and recoverable metamaterials made of brittle polymeric base materials can be found with the aid of Bayesian machine learning methods (Fig. 7).[110] Generative methods have the ability to create plenty of new designs with different structures and even better mechanical performance compared to those in the training set, suitable for not only composite design,[164] but also topology optimization.[165–167] Mao *et al.* harnessed GANs to acquire hundreds of designs of 2D periodic units in architected materials that approach the Hashin-Shtrikman upper bounds and at the same time attain desired crystallographic symmetries and porosities.[115] Other work reported the development of

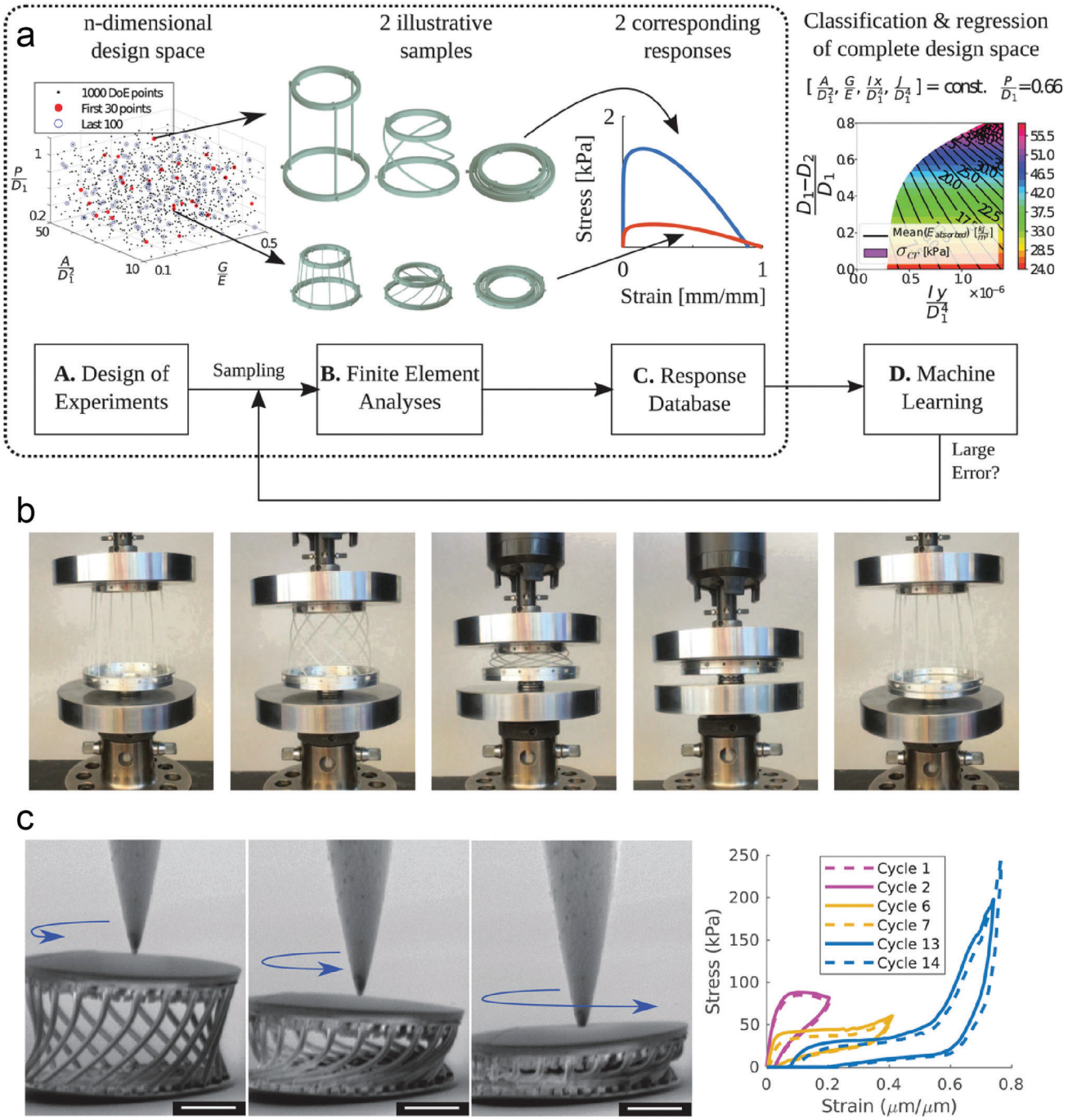

Fig. 7 Data-driven design of supercompressible and recoverable metamaterials using Bayesian machine learning. (a) Workflow of the data-driven design approach of supercompressible metamaterials. (b and c) Mechanical testing of the obtained designs of (b) a recoverable and highly compressible metamaterial produced by fused filament fabrication using polylactic acid, and (c) a monolithic metamaterial manufactured by two-photon nanolithography (scale bars, 50 μm) (Licensed under CC-BY).[110]

a semi-supervised approach to design architected materials using GNNs and the analogy between architected materials and graphs, that is, truss elements to edges, and truss pin joints to nodes.[168] Graph connectivity and the load levels of a small fraction of nodes are fed as input to the GNNs that can predict the distribution of the load levels of the remaining nodes, and then the GNN model is integrated with a design algorithm to engineer the topological structures of the architected materials.

Development of new computational methods

Data-driven approaches, developed for computational mechanics and materials analysis, are aimed to solve mechanics problems in which large datasets of material behaviors are

available while governing equations or parameters for standard computational methods are elusive.[70–73,77,78] Recently, the integration of data-driven frameworks with ML algorithms have offered new perspectives for computational approaches for modeling mechanical phenomena of materials at multi-level scales.

For instance, in order to solve nonlinear heterogeneous structure problems, neural networks have been used in a decoupled computational homogenization method where the effective strain-energy density is first computed at discrete points in a macroscopic strain space and then interpolated on RVEs.[76] Inspired by the previous method, a data-driven framework aiming to model and design new composite material systems and structures has been built, accompanied with a method called self-consistent clustering analysis that make the framework applicable to materials problems involving irreversible deformation.[78] Moreover, Liu *et al.* reported a data-driven method called deep material network, which is developed for structure–property predictions of heterogeneous materials under the effects of nonlinear, failure and interfacial behaviors.[169–172]

Wang and Sun leveraged RNNs and the concept of directed graph to address the issues on the linkages between multi-scale models of porous media using a recursive data-driven approach, where the databases generated from smaller-scale simulations are used to train RNN models at larger scales (Fig. 8).[173] They also implemented reinforcement learning to generate traction–separation laws for materials with heterogeneous microstructures.[174] Capuano and Rimoli developed a new type of finite elements called "smart elements" in which ML models provide force predictions based on the elements' states, circumventing the computation of internal displacement field and the need for numerical iterations.[175] Chan *et al.* reported an unsupervised approach that combines techniques such as topology classification, image processing, and clustering algorithms to promptly identify and characterize microstructures, including grains in polycrystalline solids, voids in porous materials, and micellar distribution in complex solutions (Fig. 9).[176] In a recent work by Samaniego *et al.*, deep neural networks based on the variational form of the boundary value problems were implemented as solvers for partial differential equations (PDEs) in various solid mechanics problems, using a fundamental idea that the energy of the system to be minimized can be naturally treated as a loss function for the neural networks.[177]

Perspectives

A straightforward benefit ML brings to materials and mechanics researches is promoting the efficiency of materials designs *via* experiments and simulations. Exploring a massive design space of novel materials is often intractable for brute force approaches and too complicated to achieve using physical intuition. Instead, ML-based design approaches can incorporate materials and mechanical features during the preprocessing of input data,

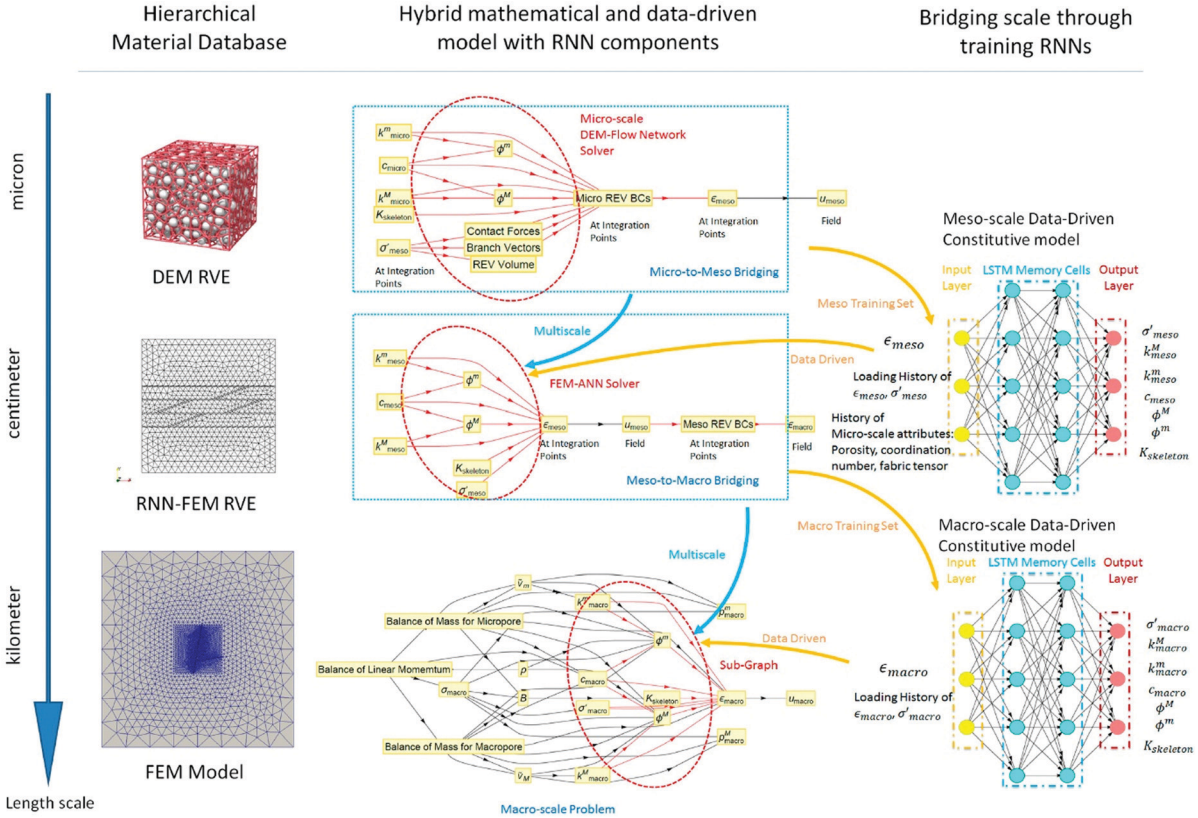

Fig. 8 A multi-scale multi-physics framework for poromechanics problems driven by directed graph representation and recurrent neural networks (Reproduced with permission.[173] Copyright 2018 Elsevier).

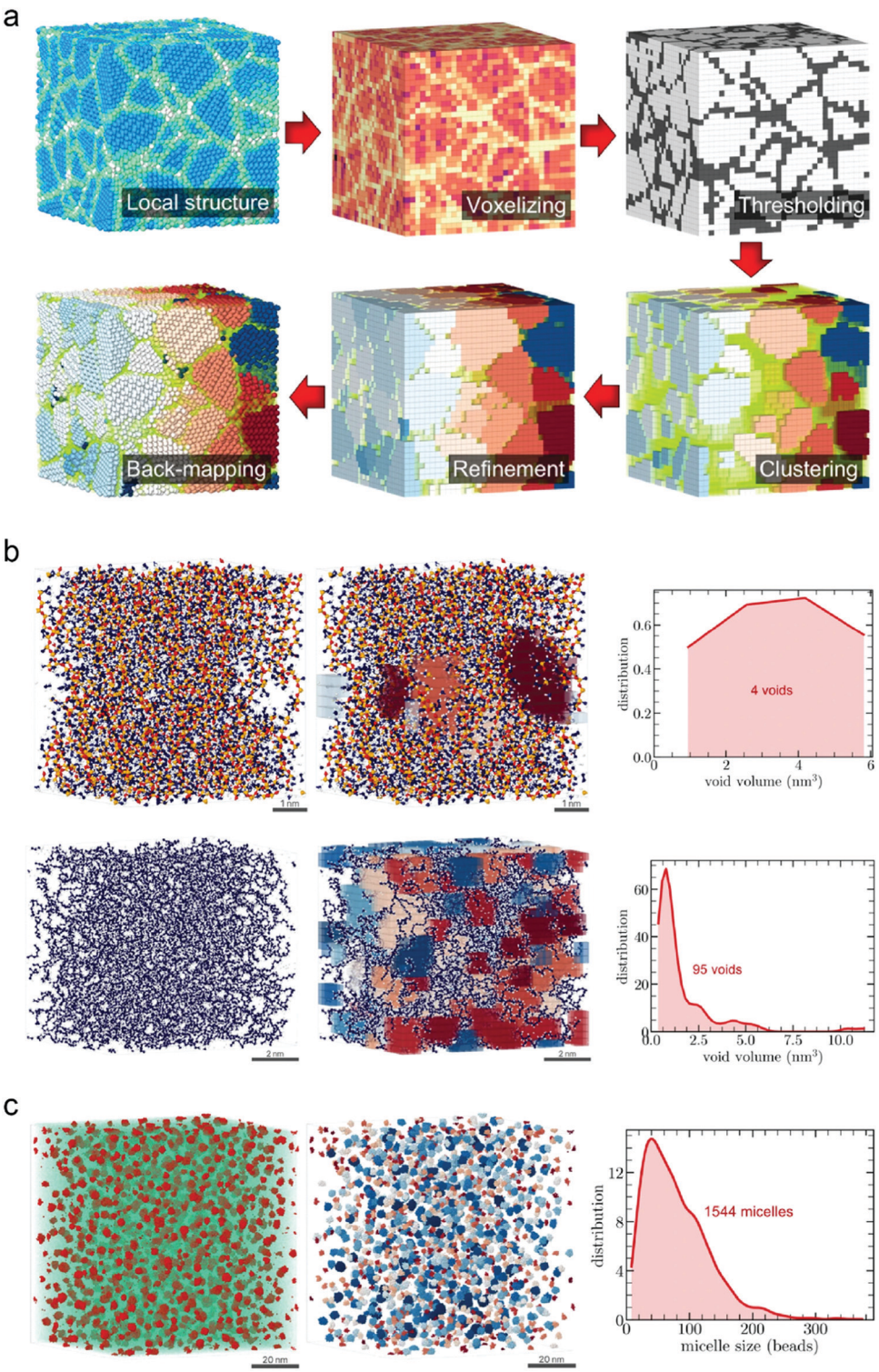

Fig. 9 An unsupervised approach for the identification and characterization of microstructures in 3-D samples of various material systems. (a) A workflow for autonomous microstructural characterization of 3-D polycrystalline solids. (b and c) Results of the ML-based microstructural analysis method on the analysis of (b) voids in porous materials and (c) micellar distribution in complex solutions (Licensed under CC-BY).[176]

learn the relationship between materials structures and mechanical behaviors during training, and provide targeted designs using the trained models. It should be pointed out that ML algorithms may not necessarily be beneficial when dealing with material problems in which the overall cost of training and design procedures is more expensive than standard approaches. A promising way to elevate the performance of ML-based methods in those problems is to encode scientific knowledge not only in data preprocessing but also in

neural networks architectures. In this regard, recent development in physics-guided ML frameworks, such as physics-informed neural networks (PINNs) in which governing equations in the form of PDEs are incorporated into loss functions,[178] offers new perspectives for the integration of ML and mechanical materials design.

ML approaches that can discover new physics may have a broad application in materials and mechanics researches. It has shown that ML can be trained to learn symbolic expression of physical laws. Well-known physics concepts including Hamiltonian, Lagrangian are predicted by symbolic regression.[179] Brunton *et al.* revealed governing equations underlying a dynamical system with ML algorithms.[180] Recent ML work using GNN has shown that the algorithms are capable to discover new analytical solutions for dark matter mass distribution.[181] These works derived governing equations in a unique way and may offer a potential new direction for understanding the mechanisms and mechanical behaviors of various materials.

As summarized in this review, most of current researches focus on applying ML algorithms to solve materials and mechanics problems. Yet, it is worth pointing out that mechanical insights also have the potential to facilitate the development of ML. Geiger *et al.* showed that loss landscape of deep neural networks can be interpreted with a paradigm based on jamming transition.[182] Inspired by information process in natural neural networks, spike neural networks (SNNs) transmit sparse and asynchronous binary signals between neurons which incorporates time into deep learning networks. As a consequence, SNNs have exhibited favorable properties including low power consumption, fast inference, and event-driven information processing.[183] Despite the popularity of ML systems, they are arguably treated as ''black boxes'' due to the difficulty of inspecting how and why those algorithms can make accomplishments. The known knowledge in mechanics and materials science may help us understand the mechanisms behind ML algorithms and develop new learning techniques that can tackle challenging problems in materials design, such as design of hierarchical structures or multifunctional materials with desired overall performance of a set of material properties.

So far, the potential of using ML in design of mechanical materials has not been fully exploited yet with opportunities and challenges lying ahead to be explored and overcome. It is promising that ML-based approaches will revolutionize the way we understand and design materials.

List of abbreviations

ABBREVIATION	MEANING
2-D	Two-dimensional
3-D	Three-dimensional
AI	Artificial intelligence
ANN	Artificial neural network
BL	Bayesian learning
BP	Back propagation
cGAN	conditional generative adversarial network
CNN	Convolutional neural network
DL	Deep learning
DT	Decision tree
FEM	Finite element method
FFNN	Feedforward neural network
GAN	Generative adversarial network
GCN	Graph convolutional network
GD	Gradient descent
GNN	Graph neural network
GPR	Gaussian process regression
GRF	Gaussian random field
GRU	Gated recurrent unit
LASSO	Least absolute shrinkage and selection operator
LIR	Linear regression
LOR	Logistic regression
LSTM	Long short-term memory
MD	Molecular dynamics
ML	Machine learning
MLP	Multilayer perceptron
MOF	Metal-organic framework
MP	Materials Project
NLP	Natural language processing
PDE	Partial differential equation
PINN	Physics-informed neural network
POD	Proper Orthogonal Decomposition
PR	Polynomial regression
RF	Random forest
RL	Reinforcement learning
RNN	Recurrent neural network
RVE	Representative volume element
SNN	Spike neural network
SVR	Support vector regression
VAE	Variational autoencoder

Conflicts of interest

The authors declare no conflict of interests.

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