Artificial Intelligence in Materials Modeling and Design

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Abstract

In recent decades, the use of artificial intelligence (AI) techniques in the field of materials modeling has received significant attention owing to their excellent ability to analyze a vast amount of data and reveal correlations between several complex interrelated phenomena. In this review paper, we summarize recent advances in the applications of AI techniques for numerical modeling of different types of materials. AI techniques such as machine learning and deep learning show great advantages and potential for predicting important mechanical properties of materials and reveal how changes in certain principal parameters affect the overall behavior of engineering materials. Furthermore, in this review, we show that the application of AI techniques can significantly help to improve the design and optimize the properties of future advanced engineering materials. Finally, a perspective on the challenges and prospects of the applications of AI techniques for material modeling is presented.

Highlights

- We present an up to date review of the application of artificial intelligence in materials modeling and design.
- We comprehensively discuss past and recent applications in modeling and design of polymers, metals, ceramics and other materials.
- We identify current research focal points, challenges, and opportunities for the application of artificial intelligence in materials modeling and design.

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Contents

1 Introduction

Computer, as an indispensable tool in modern lives, has evolved in a very stunning pace and it is gradually taking the place of humans in many fields. The ever-increasing computing power and storage capacity have made the use of computers for many complicated tasks and systems very attractive. The use of computers with high computing power and storage capacity can help humans to handle large and messy data sets with a good level of precision. Recent advances in the field of computer science and technology have equipped modern computers with the abilities and skills of "self-teaching" and "self-learning" like humans [1-3]. One of the most significant and current discussions in the field of computer science is artificial intelligence (AI). Many of the well-known AI techniques such as cognitive intelligence (CI), machine learning (ML) and deep learning (DL) are fast becoming an essential component for a wide range of modern technologies [4, 5]. For example, AI techniques are widely used in different fields such as genomics [6, 7], drug discovery [8, 9], automation [10] and financial markets analysis [11].

As one of the most famous branches of AI, ML is the science of getting computers to act like humans without being explicitly programmed [12]. It is usually employed to obtained hidden patterns in complicated systems through a training process in which a large amount of noisy data is given as input to be learned [13, 14]. ML can be classified into supervised learning where the machine learns from known data and unsupervised learning where the machine finds

patterns in data without assistance and reinforcement learning. For the latter, the machine is designed to make guesses at solutions and is "rewarded" for providing correct answers [15]. The typical working manner of different ML techniques is illustrated in Fig. 1.

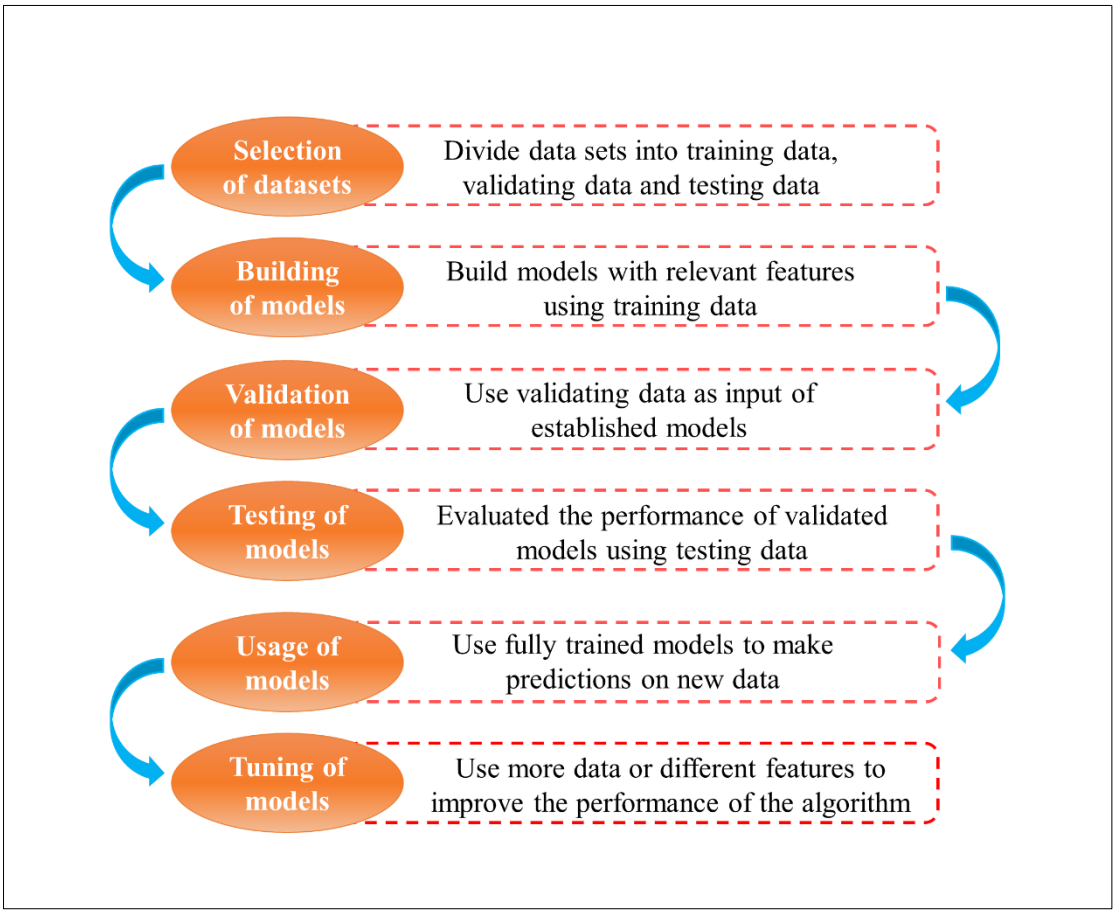

Fig. 1 The typical working manner of ML-based techniques.

One of the most challenging and active research topics in this area is searching for the optimal representation as input variables in ML models, which is often referred to as *feature engineering* [16, 17]. Feature engineering is a super-set of activities that include feature extraction, feature construction and feature selection [18]. Investigating feature engineering is a continuing concern within ML since it determines the upper limit of proposed models and is fundamental to the effective application of ML. In addition to feature engineering, algorithm development is another important aspect of ML. Studies over the past few decades have provided several basic ML algorithms including decision trees [19], naive Bayesian classification [20], K-nearest neighbor (KNN) [21], linear regression [22], support vector machine (SVM) [23], logistic regression [24], and artificial neural networks (ANN) [25]. A detailed comparison of the various features of these algorithms is presented in Table 1. The recent advances in ML have facilitated the development of self-driving cars, practical speech

and face recognition, e-mail spam detection, and a vastly improved understanding of the human genome [26-32].

DL, as an extension of ML, originates from the ANN approach, in which feedforward neural networks combined with many hidden layers are regarded as deep neural networks [33, 34]. DL systems make use of gradient-based optimization algorithms to adjust parameters throughout such a multilayered neural network based on errors at its output [35]. The architectures of some typical neural networks are presented in Fig. 2. And the characteristics of these neural networks are compared in Table 2. In comparison to ML, DL techniques that explain the vanishing effects of gradient [36] are most suitable for raw high-dimensional data, however, DL techniques suffer from certain drawbacks – they are time-consuming and data-demanding [37]. Similar to ML, DL has also shown great potential in the field of image recognition, video games, structural engineering, chemoinformatics and material science [38-41].

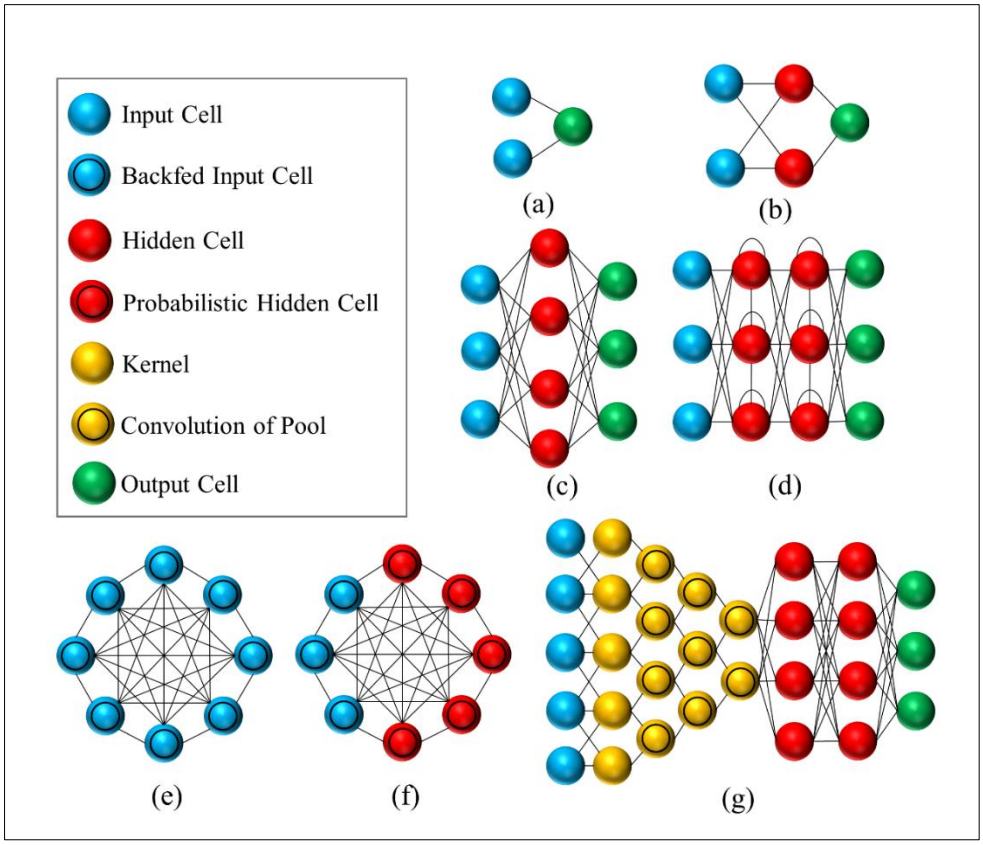

Fig. 2 Representation of architectures of some basic neural networks. (a) Perceptron neural network (PNN); (b) Radial basis neural network (RBNN); (c) Back propagation neural network (BPNN); (d) Recurrent neural network (RNN); (e) Hopfield neural network (HNN); (f) Boltzman machines (BM); (g) Convolutional neural network (CNN). (a)-(g) are constructed based on Refs. [42-48], respectively.

Table 1 Comparison among different ML algorithms

Algorithm	Type of prediction	Hypothesis	Errors	Advantages	Disadvantages	Ref.
Decision trees	Either	-	-	Simple computation; easy to understand and interpret	Easy to overfit; Neglects correlation among data	[19]
Naive Bayesian classification	Classification	-	-	Good performance for small data sets; Simple and stable algorithms	Computation of prior probabilities; Sensitive to the format of input data	[20]
KNN	Either	-	-	Simple idea and algorithm; No assumption on data; Insensitive to outlier	Large amount of computations; Poor effect for unbalanced samples	[21]
Linear regression	Regression	$y = \mathbf{w}^T\mathbf{x}$	$E = \frac{1}{N}\sum_{n=1}^{N}(y_n - y_n)$	Simple implementation and computation	Inapplicable to nonlinear problems	[22]
SVM	Either	-	-	Applicable to high-dimensional data space	Sensitive to missing data; Lack of universal solution to nonlinear problems	[23]
Logistic regression	Classification	$y = \frac{e^{\mathbf{w}^T\mathbf{x}}}{1+e^{\mathbf{w}^T\mathbf{x}}}$	$E = \frac{1}{N}\sum_{n=1}^{N}\ln(1+e^{-y_n\mathbf{w}^T\mathbf{x}_n})$	Easy to implement; Small amount of computations; Less storage occupation	Only applicable to classification problem; Easy to underfit	[24]
ANN	Either	-	-	High accuracy; Strong parallel distributed processing ability; High tolerance of noise	Long learning duration; Unreadable learning process; Large number of parameters	[25]

Notes: $\mathbf{w}$ represents the weights, $\mathbf{x}$ represents the input variables of the model and y represents the output variable. N is the number of samples, y_n is the prediction of sample n and y_n denotes the actual quantity of the sample.

Table 2 Comparison among different neural networks

Type	Known applications	Advantages	Disadvantages	Ref.
PNN	Classification	Easy to implement	Only applicable to linear systems	[42]
RBNN	Pattern recognition; Analysis of time series; Classification	Applicable to nonlinear systems; Simple algorithms; Fast convergence	Loss of information; Unable to interpret the reasoning process	[43]
BPNN	Regression; Pattern recognition; Classification; Data compression	Excellent ability to process nonlinear problems	Low training rate	[44]
RNN	Analysis of sequential data; Natural Language processing	Increasing the network depth without increasing the number of parameters	Gradient explosion and vanishing	[45]
HNN	Associative memory; Cluster analysis; Optimization calculation	Symmetric weights between connection cells	Crosstalk among patterns; Limited memorable pattern amounts	[46]
BM	Dimensionality reduction; Classification; Regression; Collaborative filtering	Symmetric weights between connection cells	Long computation duration; Sensitive to sample noises	[47]
CNN	Image recognition	Applicable to high-dimensional data; Good performance on feature classification	Need for a large number of samples; Ambiguous physical meaning	[48]

In the past few decades, with rapid advances in computing power, material science and numerical modeling, many researchers have focused on the development of new techniques to accurately and efficiently predict the properties of several important engineering materials [49-53]. For instance, quantum mechanics and density functional theory (DFT) can be used to study and predict the properties of isolated molecules, bulk solids, and materials interface [54-56]. Molecular dynamics (MD) and finite element method (FEM) can be applied to simulate materials at the nano-scale and continuum-scale [57, 58]. Multiscale models based on the meshfree method have also been developed to explore the mechanical properties of carbon nanotube (CNT) [59, 60], CNT-reinforced composites [61] and biological materials such as microtubules and red blood cells [62-64]. Numerical modeling has played a significant role in the field of material science since it can replace the repetitive process of synthesizing, manufacturing and testing materials in the laboratory with a more efficient and economical alternative with reasonable accuracy [13].

Moreover, numerical modeling can precisely narrow down the gaps in time required to solve time-consuming problems and offer more detailed information about the mechanical and fracture behaviors of materials that are sometimes difficult to observe using experimental tools. For example, the fatigue life of a material can be quickly predicted using numerical modeling but cannot be readily obtained using experimental measurements since the actual duration of the fatigue process is quite long [65]. With the help of numerical modeling, researchers can learn about the constitutive relationship of a material, based on which improvement and optimization can be made to enhance any desired mechanical properties of the material. Recently, an emerging trend in computational mechanics and material science research is the combination of the existing numerical modeling methods with AI techniques [66-72]. Traditional material science is usually advanced based on accumulated experience and summarized rules. The recent advances in numerical modeling make the systematic acquisition of a large amount of data easier, while at the same time making the analysis, hypothesizing and prediction of patterns in the acquired data more complicated. For example, the factors influencing the hydration process of cement-based materials are too numerous to be considered together, thus making it difficult to propose a common rule that controls the hydration process. The emergence of AI techniques offsets this deficiency to a large extent.

Over the past decades, rapid advances in AI techniques and relevant data science have promoted modern material modeling into the big data era. The application of AI techniques can be categorized into two types of problems [13]. One is referred to as a *forward modeling problem* in which the structure (e.g., atomic structure, crystal structure, topological structure)

of the material is given and the properties are controlled by physical laws such as quantum mechanics, thermodynamics, and solid mechanics. The other is referred to as an *inverse modeling problem* in which the structure of a material is generated based on the required properties. Common forward modeling problems, such as predicting material properties and constructing constitutive relationships, can be numerically calculated and analyzed using existing modeling tools such as DFT, MD, FEM and meshfree methods in combination with AI techniques such as ML and DL. Compared with the forward modeling problems, inverse modeling problems such as the design and optimization of material are more dependent on the use of AI techniques as there is no physics-based modeling tool that can solve inverse design problem except for trial and error method based on the knowledge and experience of the researcher. AI techniques are capable of accelerating the trial and error process, and able to explore all possible design space with satisfying accuracy. Therefore, AI techniques have been perceived as a promising tool for the design, optimization, and digital manufacturing of advanced engineering materials for sustainable application in modern technologies such as smart vehicles, robotics, and healthcare.

In this review article, we discuss the recent developments in the application of AI techniques to the field of material modeling. Here, the focus will be on the application of AI techniques to predict and optimize the properties of different types of materials as well as AI-assisted design of materials with desired properties. We review several algorithms and recent studies applying these algorithms to material modeling. Lastly, we concluded with a summary and prospects of this interdisciplinary field.

2 Application of AI techniques for modeling of polymers and their composites

Numerous literature has focused on the different applications of AI techniques on the modeling of polymers and their composites. A list of recent studies applying AI techniques to polymer modeling is shown in Table 3. Among these applications, the most important and greatly mentioned aspect is the prediction of polymer properties while mechanical properties are the most studied [73-79]. Prediction procedure usually consists of a training process, testing the performance of models, adjusting the parameters and weights, and a predictive process using the optimized and trained model to predict new solutions.

Pidaparti and Palakal [80] proposed a BPNN model to predict the nonlinear stress-strain behavior of graphite-epoxy laminates based on 959 data points. The network used in this work

had one input layer with three nodes (e.g., fiber-angles, initial stress, and incremental stress), two middle layers, and one output layer with one node (e.g., total strain). Trebar et al. [81] used a multilayer PNN to predict the mechanical properties of elastomers. In this study, rheological parameters such as minimum torque, maximum torque and scorch time in the vulcametric curve were treated as input variables while mechanical parameters such as hardness, various moduli of elasticity, elongation at break and tensile strength were used as out variables. Jiang et al. [82] adopted an ANN model to predict the mechanical and wear properties of short fiber reinforced polyamide composites. Two datasets were used in this work to train the network with material compositions, testing condition and the manufacturing process being the input variables. The output variables included wear characteristics and mechanical properties. Studies on glass transition temperature [83] and dielectric constant have also been mostly reported.

Table 3 Recent studies on applying AI techniques to model polymers and their composites.

Type	Materials	Methods	Input variable(s)	Output variable(s)	Optimization strategy of training process	Number of samples	Ref.
Predictive	Graphite-epoxy laminates	BPNN	Fiber-angles, initial stress and incremental stress	Total strain	Mean normalization	959 data points for training and	[80]
	Elastomers	Multilayer PNN	Rheological parameters	Mechanical parameters	Levenberg-Marquardt backpropagation minimization algorithm	18649 samples for hardness dataset and 4072 samples for tensile testing	[81]
	Polyamide composites	ANN	Material composition, testing condition and manufacturing process	Wear characteristics and mechanical properties	Powell–Beale conjugate gradient algorithm, gradient descent algorithm; scaled conjugate gradient algorithm; BFGS quasi-Newton method and Levenberg-Marquardt algorithm	101 samples for wear characteristics and 93 samples for mechanical properties	[82]
	Polymers	Genetic algorithm	Several descriptors	Glass transition temperature	Multiple linear regression	60 samples for training and 20 samples for predicting	[84]
	Polymers	BPNN	Several descriptors	Dielectric dissipation factor	Multiple linear regression	91 samples for training	[85]
Design and optimization	Polymers	Genetic algorithm	Combination of bandgap and total dielectric constant	Optimal polymer structures	-	150000 possible systems	[86]

Type	Materials	Methods	Input variable(s)	Output variable(s)	Optimization strategy of training process	Number of samples	Ref.
	Polymers	Genetic algorithm	Refractive index, glass transition and thermal decomposition temperatures and solubility in standard solvents	Polymer structures with satisfactory properties	-	Over 4000 unique structures	[87]
Descriptive	Fiber-reinforced plastic plate	Multilayer PNN	Depth, width, modulus of elasticity, tensile strength of plate and concrete	Bond strength	Backpropagation algorithm	-	[88]
	Polyacrylonitrile nanofibers	Multilayer PNN	Polymer concentration, applied voltage and the nozzle-collector distance	Fiber diameters	Scaled conjugate gradient backpropagation algorithm	-	[89]
	Polyurethane	ANN	Temperature	Dynamic moduli and damping factor	Backpropagation algorithm	-	[90]

Chen et al. [84] investigated a descriptor-based quantitative structure-property relationship model for the prediction of the glass transition temperature of polymers. The results showed that the glass transition temperature depends on several different descriptors and the 7-variable model was estimated to have the best training performance. Yu et al. [85] constructed a quantitative structure-property relationship model to predict the dielectric dissipation factor of polymers using BPNN. Several models with a different number of descriptors were developed and the 6-descriptor model was verified to perform best.

AI techniques are also reported to be applied in the field of polymer design and optimization. Unlike the predictive model, the design and optimization process requires an inverse thinking pattern. Although it is possible to cover all the design space using a brute-force enumeration, it is essentially infeasible in polymer design since it is a waste of computing resources. Therefore, a lot of attempts have been made to find an efficient way of obtaining polymers with desired properties. For instance, Mannodi-Kanakkithodi et al. [86] presented a new development in the field of polymer design by proposing a genetic algorithm to optimize the polymers given the desired properties. The idea is illustrated in Fig. 3. To demonstrate and validate the proposed algorithm, initial research was performed on polymers with 8 different repetitive chemical building blocks and 6 different combinations of bandgap and total dielectric constant are chosen as the targets. Results compared with the enumeration list showed that this approach indeed obtained several optimal solutions. Venkatraman and Alsberg [87] presented a machine learning strategy for the rapid design of new polymeric materials satisfying multiple desirable properties. In their study, the desired properties were set as refractive index, glass transition and thermal decomposition temperatures and solubility in standard solvents. All the proposed structures were evaluated in terms of desired properties which were obtained using ML models. After selection, all the remained candidates passing criterion were further analyzed using DFT approaches.

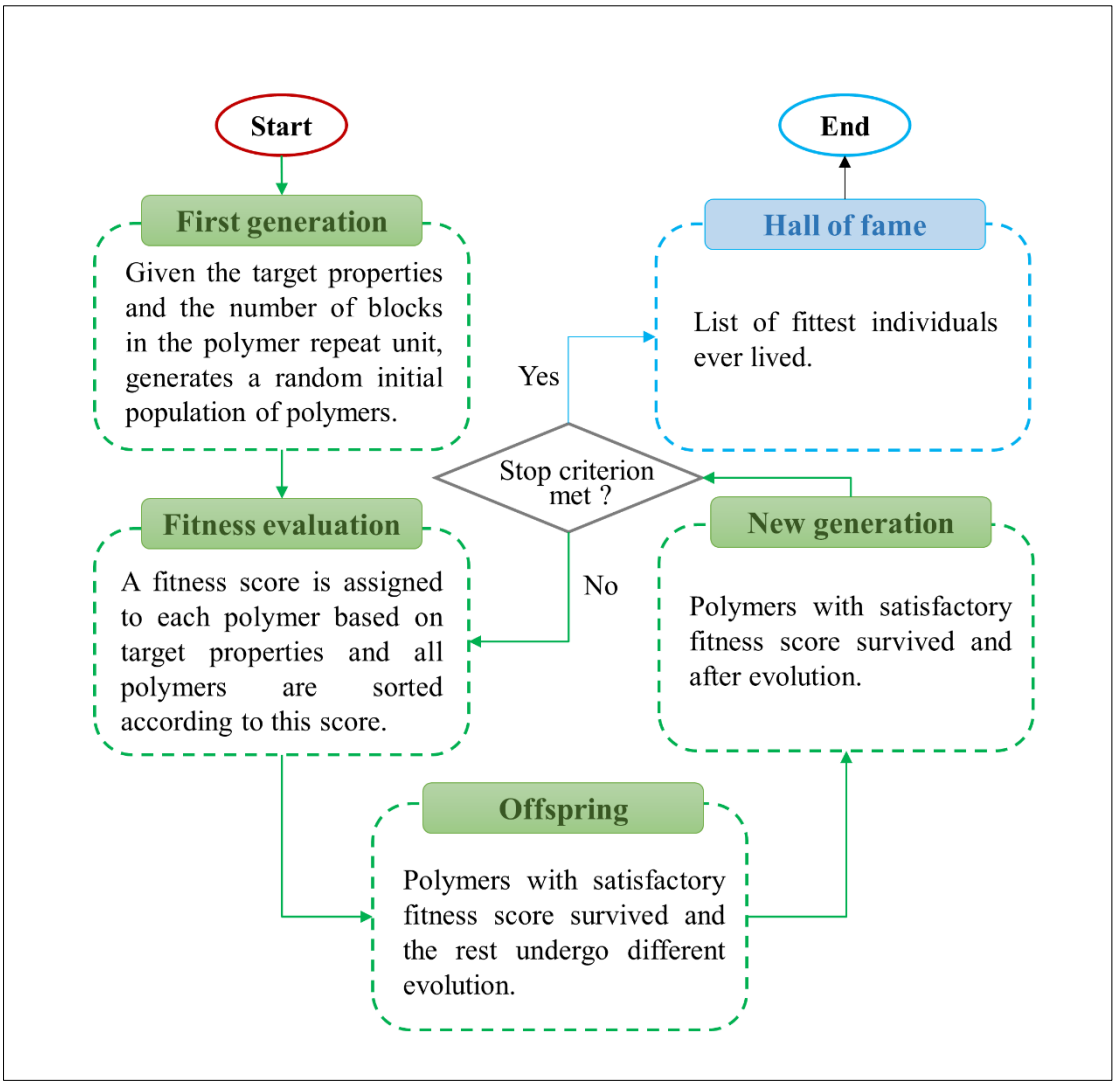

Fig. 3 The steps involved in the genetic algorithm leading to the direct design of polymers (modified after Ref. [86]).

In addition to the above-mentioned application, another relevant topic involves the use of AI techniques to establish a descriptive relationship between parameters and properties based on data of experiments conducted by previous researchers. Park et al. [88] proposed a multilayer perceptional model to correlate several parameters with the bond strength of a fiber-reinforced plastic (FRP) plate based on the previous research data. The variables including depth, width, modulus of elasticity, the tensile strength of FRP plate and the compressive strength, tensile strength and width of concrete (to be reinforced with the FRP plate) were used as input layers. And the developed BPNN was learned to be converged within the range of 0.001. Nasouri et al. [89] investigated the average diameter of electrospun polyacrylonitrile nanofibers using a multilayer PNN. Three important electrospinning factors were studied as input variables including polymer concentration, applied voltage and the nozzle-collector distance. Their

results showed that second-order polynomial regression between input and output exhibited a high regression coefficient. Kopal et al. [90] used ANN techniques to model the temperature dependence of dynamic mechanical properties and visco-elastic behavior of thermoplastic polyurethane over a wide range of temperatures. Here, temperature was used as the input variable to estimate both dynamic moduli and damping factor.

3 Applications of AI techniques for modeling of metals and their composites

In this section, a review of recent studies applying AI techniques to the computational modeling of metals and their composite is presented. Like polymers, the application of AI techniques on the metals and their composites can also be categorized into predictive modeling, design and optimization, and descriptive modeling. Unlike polymers, the mechanical properties of metals and their composites are attracting more attention [91-102] and a large number of literature focusing on the predictive modeling of mechanical properties of metals are given in Table 4.

The most common mechanical properties being predicted are static strength (e.g., tensile strength, compressive strength, shear strength and bending strength). For instance, Altinkok and Koker [103] applied a BPNN to predict the bending strength of Al_2O_3/SiC particulate reinforced aluminum. The particle size of the reinforced phase was treated as the input layer and bending strength served as the output layer. Experiments were also conducted to provide training and testing data sets of the neural network. Results showed that bending strength was inversely related to the reinforced SiC particle size. Besides, Altinkok and Koker [104] evaluated the performance of different training algorithms by checking the system accuracy for each training algorithm at the end of learning. Results showed that Levenberg-Marquardt learning algorithms made the best prediction for bending behaviors of aluminum metal matrix composites compared with quasi-Newton, resilient backpropagation and variable learning rate backpropagation algorithms.

Jayaraman et al. [105] investigated the influences of friction stir welding process parameters on the tensile strength of A356 cast aluminum alloy. Three input nodes corresponding to 3 process parameters (e.g., rotational speed, welding speed, axial force) were investigated and rotational speed was found to have the greatest influence on tensile strength. Chen et al. [106] adopted ANN to predict the strength of particulate reinforced metal matrix composites and understand how these values were related to the underlying composite structure. In this work,

both classification and regression networks were trained from the results of finite element simulations. Input variables were classified into 3 categories (e.g., homogenized material parameter, results of elastic simulation and highly strained volume fraction in the limit state). The obtained networks convinced that the highly stressed volume fractions, in particular the ones in the binder phase, had a significant influence over ultimate strength. Except for static strength, tribological behaviors of metallic materials also draws a lot attention.

Kavimani and Prakash [107] adopted Taguchi coupled ANN technique to predict the tribological behaviors of reduced graphene oxide reinforced magnesium metal matrix composite. Specific wear rate characterizing the tribological behaviors of the composite was used as the output variable and 4 parameters were treated as input variables including weight ratio of reinforcement, load, sliding velocity, and sliding distance. Results indicated load exerted more contribution in determining the specific wear rate of composite. Genel et al. [108] established a multiple-layer feed-forward ANN to model the tribological behavior of short alumina fiber reinforced zinc-aluminum composites. Fiber volume, load, and fiber orientation were fed into the neural network as input variables to predict the specific wear rate. It could be concluded that ANN was a good analytical tool that has potential use in the field of wear behavior for the design of metal–matrix composites if properly used. Another remarkable application of AI techniques involves predicting the creep and fatigue behaviors of metallic materials. Gupta et al. [109] reported an ANN model for predicting the creep response of a rotating Al-SiC_p composite disc operating at elevated temperature. The creep response was output based on several combinations of particle size, particle content, and temperature. The results predicted by ANN were slightly overestimated compared to the corresponding analytical values so that some factor of safety should be taken into consideration.

Maleki and Kashyzadeh [110] developed an ANN model to predict the fatigue behavior of CK45 mild steel. Input layers consisting of stress amplitude and coating thickness were fed into the neural network to predict the fatigue life. Training data were obtained by performing fatigue life tests while predictive data were compared with FEM results. Results suggested that the ANN model outperformed FEM. Zhang et al. [111] used a neuro-fuzzy-based ML method for predicting the high cycle fatigue life of laser powder bed fusion stainless steel 316L. Two models employing different variables as the inputs were implemented. The process-based model adopted the processing and post-processing parameter as the inputs while the property-based model used ultimate tensile strength and elongation to failure as the inputs.

In addition to mechanical properties, other performances of metallic materials have also been

evaluated using AI techniques in recent decades. Sivasankaran et al. [112] analyzed the workability behavior of Al-SiC powder metallurgy metal matrix composites using an ANN model. The input parameters of the ANN model were the preform density, the particle size, the percentage of reinforcement and the applied load and the output variable is workability. Ji et al. [113] developed an ANN model to predict the hot deformation behavior of the ultrahigh strength steel. The inputs of the neural network were strain, strain rate and temperature, whereas flow stress was the output. The developed feed-forward backpropagation ANN model was trained with the Levenberg–Marquardt learning algorithm. The performance of the ANN model was evaluated using a wide variety of standard statistical indices.

Kautz et al. [114] employed a deep neural network to predict the thermal conductivity of the uranium-molybdenum system. An input vector contained the following information: molybdenum concentration and uranium enrichment at both the beginning and end of life, ^{235}U depletion and measured depletion, fission density and measured fission density, fission power, surface heat flux, neutron, and average advanced test reactor loop temperature. Yekta et al. [115] applied a hybrid ANN and genetic algorithm to predict the hysteresis loop and magnetic properties of Fe-48Ni. In this case, the thickness of samples, annealing temperature, holding time and field strength were treated as the network inputs and the magnetization as the output. The major conclusions of this research showed that ANNs as powerful computational techniques in the modeling of nonlinear systems could be reliably used in the prediction of hysteresis and magnetic properties of alloys.

Table 4 Recent studies applying AI techniques to predict mechanical properties of metallic materials

Mechanical properties	Material	Methods	Parameters of neural network	Affecting parameter(s)	Optimization algorithm for the training process	Number of samples	Ref.
Bending strength	Al_2O_3/SiC particulate reinforced aluminum matrix composite	BPNN	3 layers with learning rate of 0.2 and momentum coefficient of 0.8	Reinforced particle size	Gradient descent learning algorithm	15 samples	[103]
Tensile strength	A356 cast aluminum alloy	BPNN	3 layers	Process parameters	Levenberg-Marquardt algorithm	-	[105]
Ultimate strength	Particulate reinforced metal matrix composites	ANN	4 layers	3 categories	-	500 samples	[106]
Specific wear rate	Reduced graphene oxide reinforced magnesium metal matrix composite	ANN	3 layers	Weight ratio of reinforcement, load, sliding velocity, and sliding distance	Levenberg-Marquardt algorithm	24 samples for training and 3 samples for testing	[107]
Specific wear rate or friction coefficient	Short alumina fiber reinforced zinc-aluminum composites	ANN	3 layers with learning rate and momentum coefficient increasing from 0.1 to 0.9	Fiber volume, load, and fiber orientation	Backpropagation algorithm	34 samples for training and 14 samples for testing	[108]

Mechanical properties	Material	Methods	Parameters of neural network	Affecting parameter(s)	Optimization algorithm for the training process	Number of samples	Ref.
Stress and strain rates	Al-SiC_p composite	ANN	4 layers with learning rate of 0.05 and momentum coefficient of 0.65	Reinforcement size, content, and temperature	Backpropagation algorithm	6 data sets for training	[109]
Fatigue life	CK 45 mild steel with nickel coating	ANN	4 layers with learning rate of 0.13, 0.14, 0.145 and 0.15	Stress amplitude and coating thickness	Backpropagation algorithm	-	[110]
Fatigue life	Stainless steel	ANN	4 layers	Processing parameters and tensile properties	-	139 samples	[111]

4 Applications of AI techniques for modeling of ceramics and their composites

In this section, a concise review on the application of AI techniques for predicting the mechanical properties of ceramics and their composites is presented. The specific properties of interest are micromechanical behavior, electric conductivity, thermoelectric properties, and permittivity and diffusion coefficients. Rao and Mukherjee [116] presented a novel approach using ANN to predict micromechanical behaviors of ceramic matrix composites. The training examples for the network have been generated through an accurate micromechanical finite element analysis that simulated the interfacial debonding and sliding realistically. In their work, the stress and the corresponding strain at a point along with the desired small increment in stress were provided as inputs and the corresponding increment in strain served as output. Rao continued his work and proposed a genetic algorithm based BPNN to simulate the stress-strain response of Al_2O_3/SiC ceramic matrix composites [117]. The genetic algorithm was used to obtain the weights for BPNN. The newly proposed model was capable of predicting the stress-strain relationship for a new interface shear strength even with this limited information.

Wen et al. [118] applied an ANN model to investigate the relationship between the composition content and the properties of slag glass-ceramic. The investigation showed that the ANN had an excellent prediction performance once data sets reflected the relationship between the composition and property. Scott et al. [119] developed ANNs for the prediction of the properties of ceramic materials. Multi-layer perceptron ANNs were trained using the backpropagation algorithm and utilized data obtained from the literature to learn composition-property relationships between the inputs and outputs of the system. The trained networks used compositional information to predict the relative permittivity and oxygen diffusion properties of ceramic materials. Xu et al. [120] used a feed-forward, multilayer PNN model with eight hidden layers and 12 neurons to predict the corrosion behavior of Ni-SiC composite coatings deposited by ultrasonic electrodeposition. The effect of process parameters (e.g., ultrasonic power, SiC particle concentration, and current density) on the weight losses of Ni-SiC composite coatings were investigated.

Guo et al. [121] adopted ANN to predict and analyze the electrical properties of piezoelectric ceramics. The input variables consisted of dopant content and temperature and output were electrical properties. The same set of results of piezoelectric ceramics samples were analyzed

using a backpropagation network in comparison with a multiple nonlinear regression analysis model. The results obtained revealed that the ANN model was much more accurate than multiple nonlinear regression analysis model. The importance of design and optimization of ceramics and their composite combined with AI techniques is also not to be ignored. Deng et al. [122] proposed a combined model of orthogonal experiment design and backpropagation ANN to solve multi-objective and multi-factor problems caused by the preparation of alumina slurry. The networks with five inputs, two outputs and a hidden layer of 11 nodes were used in this work. The optimal values with different weights of extrusion time and extrusion width deformation were obtained. The results from predicted values matched well with the experimental ones, and the average error was less than 3%.

5 Applications of AI techniques for modeling of other materials

In this part, the application of AI techniques for modeling of other materials such as cement-based materials and nanoscale materials such as carbon nanotubes will be briefly reviewed. The modeling of cement-based materials mainly focuses on the prediction of their mechanical properties [123-127]. For example, Nazari and Sanjayan [128] used SVM to predict the compressive strength of geopolymers. Five different well-known optimization algorithms including genetic algorithm, particle swarm optimization algorithm, ant colony optimization algorithm artificial bee colony optimization algorithm and imperialist competitive algorithm are implemented to find parameters of SVM. By evaluating the proposed models through their coefficient of determination and errors, it was concluded that imperialist competitive algorithm and genetic were more suitable to optimize parameters of SVM for predicting compressive strength of the considered geopolymers. Other properties are also simulated and modeled using AI techniques.

Ramadan and Nehdi [129] reported an approach to predict intrinsic self-healing in concrete using a hybrid genetic algorithm-ANN. A genetic algorithm was implemented in the network as a stochastic optimizing tool for the initial optimal weights and biases. The model inputs included the cement content, water-to-cement ratio (w/c), type and dosage of supplementary cementitious materials, bio-healing materials, and both expansive and crystalline additives. Self-healing indicated through crack width was the model output. The results showed that the proposed model was capable of capturing the complex effects of various self-healing agents on the self-healing performance in cement-based materials.

With regard to nanoscale materials, AI techniques are usually combined with FEM and MD to characterize the properties of nanomaterials. Shabani and Mazahery [130] modeled the mechanical properties of Al matrix nanocomposites. The effect of the volume fraction of the alumina nanoparticles on the mechanical properties of the Al-Si matrix composites was studied. The yield strength and tensile strength increase, but the elongation decreased with the increase in the volume fraction of the particles, indicating that increasing the volume fraction of the Al_2O_3 particles can improve the strength but degrade the plasticity of the composites.

Vijayaraghavan et al. [131] proposed an MD-based AI simulation approach to investigate the thermal transport of carbon nanotubes. In this approach, the effect of size, chirality and vacancy defects on the thermal conductivity of carbon nanotubes was first analyzed using MD simulation. The data obtained using the MD simulation was then fed into the paradigm of an AI cluster comprising genetic programming, which was specifically designed to formulate the explicit relationship of thermal transport of CNT with respect to system size, chirality and vacancy defect concentration.

6 Summary, challenges and prospects

This paper presents a concise review of recent advances in the application of AI techniques to material modeling. A brief overview of some basic ML algorithms and DL neural networks is given to illustrate the advantages and disadvantages of these types of AI methods. Following the introductory section, a review of recent studies employing AI techniques to predict and model important mechanical properties of different types of materials is presented. In the reviewed studies, AI techniques were most frequently used to predict the properties of materials. For this kind of application, the learning process is first performed on training datasets, and then the predictive process is implemented to predict specific properties. Usually, a predictive model is accompanied by a validation or testing procedure to evaluate the predictive performance of the model. As for the design and optimization problem, the genetic algorithm seems to be the most suitable tool to solve the inverse forward problem. Descriptive models are similar to a regression model where the target is to find the correlation among several parameters.

Although AI techniques show great potential in their applications to material modeling, there are still several challenges facing this emerging interdisciplinary field. For example, the

evolution of computers and computer science outpaces that of material science, which will lead to data deficiency. This deficiency not only indicates the shortage in the number of available datasets but also refers to the disunity in the data representation. The deficiency in data will inevitably hamper further developments in this important interdisciplinary field. One of the possible solutions to this issue is the establishment of general rules for constructing datasets, which is a tough and time-consuming task. The same problems exist in the usage of AI models. Presently, most ML and DL models are only applicable to a specific question under a specific environment such that every time a new problem is identified, a new model needs to be constructed, which is a huge waste of computing resources. For example, there is no acceptable generalized rule for selecting the number of neurons in the hidden layer, which will definitely influence the performance of a neural network. The best solution to this problem is to generalize the usage of models and neural networks. However, this is almost impossible at the present stage since we do not have a full understanding of how AI operates. It is necessary to advance in this direction so that the usage of models can be generalized in a unified form in the future.

Another gap existing in the current body of research works on AI-assisted materials modeling is the sparse usage of multiscale modeling techniques. As accepted by many researchers, AI techniques can perform well at each independent scale, however, more research works are needed on constructing a linkage between multiple scales. This is quite a significant problem as materials' properties are influenced by their inherent microstructures, which is similar to the idea that the overall physiological functions of the human body are influenced by the biomechanical behavior of cells. Although, some progress is currently being made on incorporating ML into multiscale modeling [132]. There is an urgent need to strengthen these linkages in order to harness the benefits of these two important methodologies for practical applications.

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