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Application of Artificial Neural Networks in Polymer Composites: A Review

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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Review Article

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ABSTRACT

Artificial neural networks (ANN), which have been a hot topic in the field of artificial intelligence (AI) since the 1980s, are widely applied these years for their strong ability in the field of nonlinear mapping, pattern recognition, robots, automatic control, biology, economy and so on. This review presents and summarizes the history of artificial neural networks, briefly introducing the application of artificial neural networks. After that, the paper focuses on an overview of research advances in neural networks for polymer composites and introduces several classical categories of applications. Finally, we look ahead to the development of neural network applications in polymer composites and provide a future outlook for the application of artificial neural network in polymer composites.

Keywords: Artificial neural networks; polymerization; material properties.

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1. INTRODUCTION

Artificial neural networks (ANN) [1] abstract the neuronal network of the brain from the information processing point of view, build a simple model, and form different networks according to different connection methods. The brief structure of the neural network is schematically shown in Fig. 1. Since the 1980s, artificial neural networks have increasingly become state of the art for their neurobiological way to finish computation. The field of artificial neural networks tries to simulate and fabricate networks and devices in the spirit of neurobiology, to solve useful computational problems of the kind that biology does effortlessly [2].

In the field of materials science, owing to their diverse structures and properties, polymers exhibit a wide range of potential applications in energy storage, biomedicine, and electronic devices. However, it is the complexity of polymer materials that make theoretical modelling and design difficult. Different types of composites are shown in Fig. 2. So, there is an urgent need for a mathematical tool to speed up calculations. For this reason, artificial neural networks play an important role in the prediction and optimization of polymer composites.

Trained by a large amount of data, artificial neural networks can accurately predict the properties of various polymer materials, such as mechanical strength, thermal conductivity, and electronic energy levels. The capability of prediction helps researchers quickly obtain the estimation of material properties. Additionally, neural networks have a wide range of applications in the synthesis of polymer materials. The synthesis of polymers is a complex process which needs to focus on many parameters such as the ratio of reactants, reaction temperature and pressure. Traditional trial-and-error methods are inefficient, while neural networks can find the best synthesis conditions and enable control of the optimization process by learning a large amount of experimental data. This method can greatly reduce the trial-and-error time and cost, and improve the synthesis efficiency and success rate.

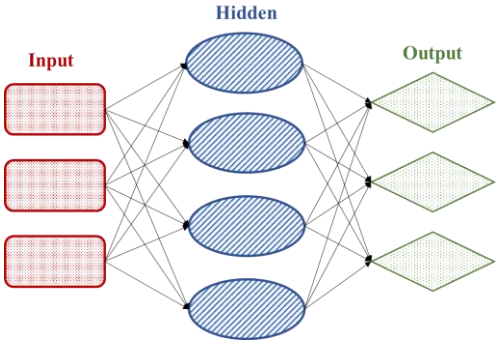

Fig. 1. Artificial neural networks [3]

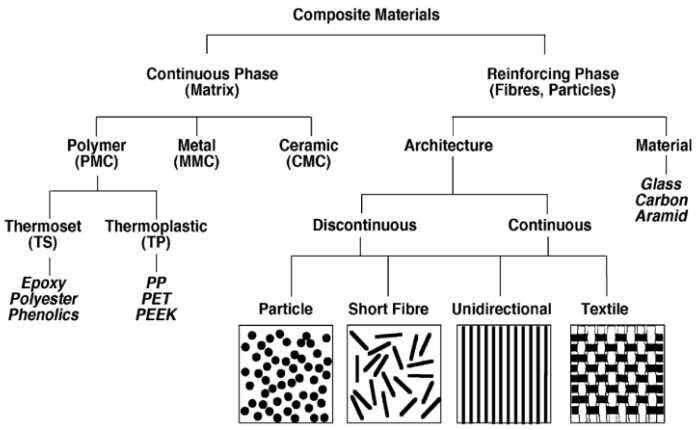

Fig. 2. The types of composites materials [4]

This paper will provide an overview of the research advances in artificial neural networks, as well as a brief review of the research advances in applying neural networks in the field of polymer science. Finally, the paper will introduce a few selected types of typical applications in polymer composites.

2. ARTIFICIAL NEURAL NETWORKS

2.1 Concepts of Neural Networks

Different from the traditional way, artificial neural networks are mathematical tools to solve complex engineering problems inspired by the biological nervous system [5,6]. The basic components of artificial neural networks are *neurons*, similar to the terminology in neuroscience [7,8]. The cells in the human brain, which are known as neurons (Fig. 3), enable us to acquire the ability to memorize, think, and respond appropriately to the things we meet.

A neuron consists of dendrites, a cell body and an Axon. Each neuron can connect with millions of neurons. When they connect, the neurons can deal with complex such as like communication and recognition at breakneck speed, which take only a few hundred milliseconds. Rigby et al. [9] proposed the use of backpropagation to train the neural networks. They investigated the time scales and feasibility of building an artificial neural network by manipulating single neurons and creating functioning synapses (Fig. 4) and then systematically changed the weight of neuronal connections. Finally, they have developed a model that can characterize the significant growth of mechanically induced neurons. Furthermore, they demonstrate that the robustness of such networks can be tested by axotomizing specific axons and then reconnecting them.

It is shown that the information among the neurons is not transmitted linearly but delivered in the neuron networks. ANNs can be defined as a massively parallel distributed processor of simple units which can store experience and knowledge and put it to use in natural ways similar to the human brain.

The basic model of ANNs is shown in Fig. 5. Each node can receive information from different inputs through connections containing weights. It will be activated by the sum of the input weighted values exceeding the threshold and passes the signal to neighbouring nodes through a transfer function. The process can be represented by this mathematical model [1]:

$$y = f(\sum_{i=0}^{n} w_i\, x_i - T) \quad (1)$$

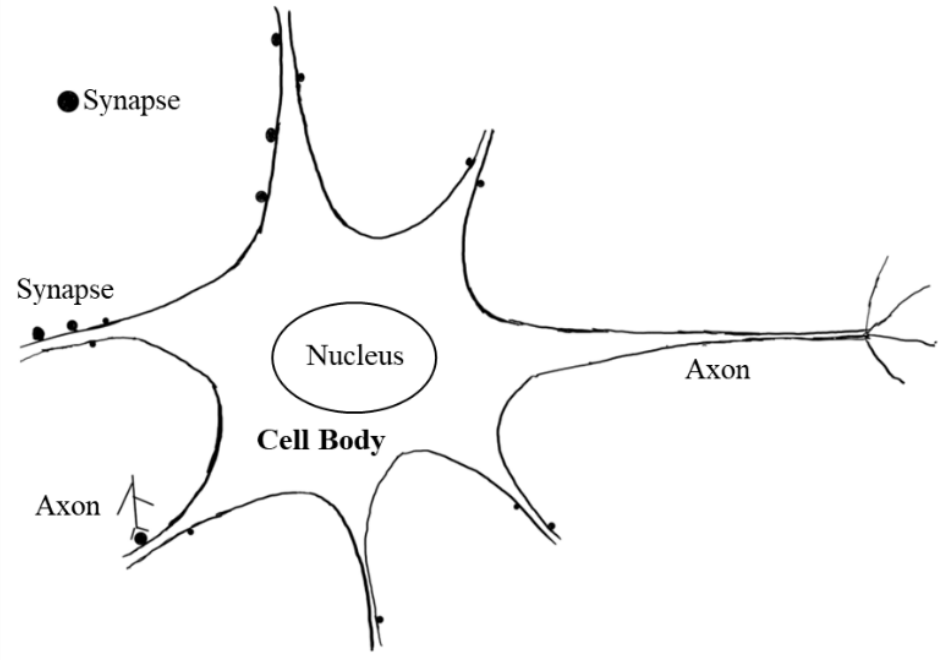

Fig. 3. A sketch of neuron

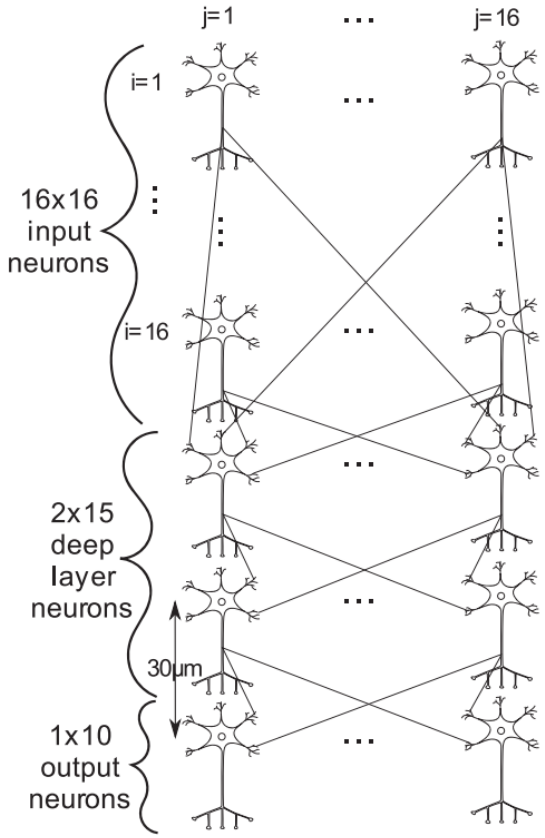

Fig. 4. The way to build a neural network [9]

In this equation, x_i is the input, w_i is the weight of it, y is the output of the node; f is the transfer function and T is the threshold value. The transfer function can be divided into line processes and nonlinear processes, which the nonlinear processes are more useful than linear ones. The simplest one is as follows (Fig. 6).

$$y = \begin{cases} 0, \dots if \sum_{i=0}^{n} w_i x_i > T \\ 1, \dots if \sum_{i=0}^{n} w_i x_i < T \end{cases} \quad (2)$$

The sigmoid function is also used for the activation function for its continuity. The curve of the function is shown in Fig. 6.

$$y = \frac{1}{1+\exp(-\beta x)} \quad (3)$$

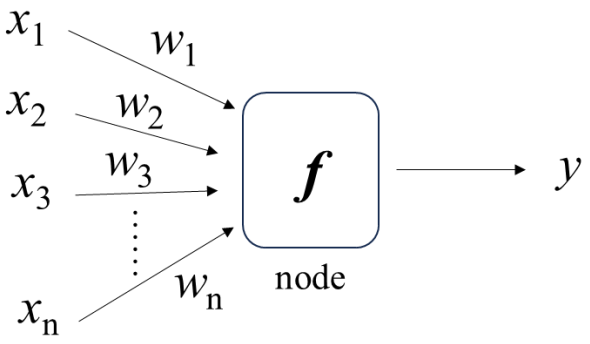

Fig. 5. The basic model of ANNs [3]

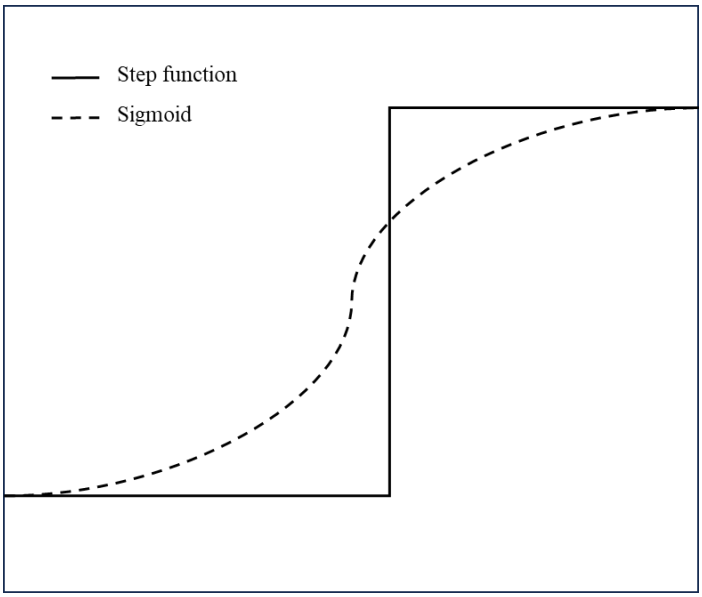

Fig. 6. Transfer function

2.2 Development of Artificial Neural Networks

The development process of the ANNs started in the 1940s. In 1943, Mcculloch and Pitts [1] found that the events and the relations of neurons can be treated using propositional logic and for any logical relational equation that satisfies a particular condition, a neural network whose behaviour agrees with its description can be found. Thus, they proposed the M-P model, which became the beginning of the research work on artificial neural networks. Based on the M-P model, Rosenblatt [10] introduced the Perceptron model which has the fundamental principles of modern neural networks in 1957. It is an M-P model with continuously adjustable weights that can classify and discriminate specific input vector patterns. This model was the inaugural neural network in the true sense of the word. Rosenblatt demonstrated that the sensors of two-layers could classify inputs. They also proposed a research direction for three-layer sensors with concealed processing elements. Rosenblatt's model encompasses some of the fundamentals of modern neural computers and represents a breakthrough in methodology and technology. A decade later, *Perceptron*, which was written by Minsky and Papert [11] in 1969, has been published to present a mathematical theory of the class of machines. The book points out that linear perception cannot simply solve the problem of classifying two kinds of linearly indivisible samples, which gave a strong hit to the artificial neural network research at that time.

After a decade-long downturn, Hopfield et al. [12] designed a model based on neurobiology, surprisingly, it was readily applicable to integrated circuits in 1982. By using integrated circuits to implement corresponding models, their asynchronous parallel processing capabilities can be used to provide fast solutions to some special classes of computational problems. Meanwhile, Hopfield has proposed a continuous neural network and taken it into application [13]. Hopfield model has galvanized a large group of scholars to study neural networks and continue to explore this field.

Kirkpatrick et al. [14] first used the SA (Simulated Annealing) algorithm to solve combinatorial optimization problems in 1983. SA algorithm is a stochastic optimization algorithm based on the Monte Carlo iterative solution strategy. The purpose is to provide an efficient approximate solution for problems with NP complexity, which overcomes the shortcomings of other optimization processes that tend to fall into local minima and the dependence on initial values. In 1986, Rumelhart et al. [15] proposed the back propagation (BP) algorithm to solve the weight correction problem of multi-layer neural networks. After that, the ability of multi-layer neural networks came into view. In 1991, Haken introduced synergy to neural networks. He believes that cognitive processes are spontaneous. In 1994, Liao et al. [16] re-examines the mathematical theory of CNNs (cellular neural networks) in-depth and

summarizes and refines a series of theoretical results.

By the 20th century, deep learning (DL), which was proposed by Hinton et al [17], made its way into the history books. Essentially, deep learning is an extension of machine learning. Deep learning is the construction of a model with multiple hidden layers and through large-scale data training to obtain a large number of representative feature information. DL break the traditional limitation of the number of layers, and the layers can be chosen according to the needs. Generative adversarial networks were introduced by Goodfellow et al. [18] in 2014, which showed an idea about the competition between two neural networks that can produce new data. Recently, deep learning algorithms have been applied to analyse big data [19].

After several decades of development, neural networks have been successfully applied in many fields such as artificial intelligence [20,21], pattern recognition [22-24], signal processing [25,26], optimization [27-29], prediction [30,31], etc. Prediction is one of the main functions of neural networks. ANNs can predict financial stability, which performs quite excellently in the economic, and management fields [32,33]. Additionally, ANNs have been used in the judgment of policymaking by predicting the probability of success or failure [34]. ANNs can also be used to predict climatic change which is a great help for people's daily production activities.

ANNs also focus on the field of medicine. Sardari et al. [35] hoped that predicting the structure of the AIDs will guide pathology research and treatment modalities. There are also applications in biological signal detection and analysis. As a type of adaptive dynamical system, artificial neural networks can be utilized for self-adaptive learning, parallelism, and distributed storage. As opposed to the traditional way of solving the problem of biomedical signal analysis, these abilities can be used to solve the problem of analysing biomedical signals in a revolutionary way, which opens up new opportunities for medical research and development.

In this section, we talk about the concept and review the development and applications of artificial neural networks. Artificial neural networks are tools to solve complex engineering problems. From 1943 to the present, the development of artificial neural networks has gone through rise, ebb, revival and flourishing. There are some popular artificial neural networks such as *Perceptron*, *Hopfield model*, *SA algorithm* and *BP algorithm* being reviewed in the chapter. As technology advances, so does artificial neural network technology. In the future, neural networks will be applied to more fields.

3. ARTIFICIAL NEURAL NETWORKS IN POLYMER COMPOSITES

Polymer composites are widely applied in various modern industries for properties like high strength, high ductility, translucency, impact resistance, etc. Polymer composites typically consist of two phases: a continuous phase and a dispersed phase [36]. According to the nature of the recruitment material classification, polymers can be divided into plastic, rubber and fibre. Different types of polymer composites can be used in various fields. Due to the complex structure and properties of polymers, it is very difficult to accurately design the structure of the polymerized material and to regulate the properties of the polymerized material. Advances in neural networks and artificial intelligence breathe new life into the polymer materials field.

One of the applications of ANNs is for the design of materials. ANNs can be trained using material data to predict the properties of new materials. By analysing data on the physical and chemical properties of the material, a model can be built to predict novel materials, such as solubility [37] and solvent activity [38]. Furthermore, it is possible to optimize the molecular structure of materials, to obtain the desired material performance by using artificial neural networks. The structure parameters of polymeric materials can be used as inputs, with material performance as outputs, to construct a neural network model. This model can then be optimized to improve the molecular structure of the polymeric material [39]. Additionally, neural networks can utilize existing functional material data for learning and predicting intriguing new materials to guide the functional design of polymer composites. The use of neural networks for model training and prediction can accelerate the development process of new functional materials and enhance the efficiency of material discovery.

Artificial neural networks are also useful in predicting the characteristics of composite materials such as mechanical properties [40] and thermal properties [41]. The density of a material can be predicted by available data of the

materials. By inputting the molecular structure parameters and composition of the polymerized material, the characteristics are compared by neural network models with the experimentally measured values, thus verifying the accuracy of the model. The mechanical properties of polymeric materials are also one of the important indicators for their application, including modulus of elasticity, tensile strength, fracture toughness and so on. The mechanical properties can be predicted by establishing a neural network model, and provide guidance for engineering applications The thermal properties of polymeric materials determine the range of applications of the materials in high and low temperature environments. By analysing data, the thermal conductivity, coefficient of thermal expansion and other performance parameters of the new material can be predicted.

There are also some applications of artificial neural networks in materials optimization. The performance of polymeric materials is affected by the formulation, and the neural network algorithm can be used to predict the optimal material formulation for a specific performance requirement based on the statistical laws of the available data. The process parameters (e.g., temperature, pressure, reaction time, etc.) of polymerized materials have an important influence on the material properties. Neural networks can predict the relationship between process parameters and material properties, and improve the properties of polymerized materials by optimizing the process parameters [42].

The application of artificial neural networks to polymeric materials brings new opportunities and challenges for research and applications in the field of materials science. By predicting material properties, optimizing molecular structures, predicting performance parameters, and optimizing material formulations and process parameters, neural networks provide new solutions for the design, development, and optimization of polymeric materials. The next chapter of the paper will review several typical applications of artificial neural networks for polymer composites.

4. APPLICATIONS OF ARTIFICIAL NEURAL NETWORKS IN POLYMER COMPOSITES

4.1 Neural Network for the Design of Materials

Design of materials focuses on the prediction and function approximation concerning materials performance. The main difficulty is to solve the relationship among composition, process and properties. In 2007, Sun et al. [43] used BP neural network to predict the properties of the lead-free solders. After obtaining the best algorithm and parameter by BP neural network, In *Striketthrough*. Bi, Sb, RE Cu were added to Sn-Ag alloy to explore the effect of the addition of different elements on shear strength, tensile strength and solidification temperature. Then 15 groups of data were selected for model training, and 3 groups for prediction. The comparison data are shown in Table 1.

Table 1 shows that the error between the experimental data and the prediction data is almost less than 5%, only one of them reaches 7% for the less experimental data available or the measuring mistake. It is clear that the predicted data are in good agreement with the experimental results.

Li et al. [37] reviewed the solubility prediction of gases in polymer based on ANNs, briefly stating the principle, progress and performance of different ANN algorithms. The paper compares the accuracy of different models (CSAPSO-BP ANN, CSAPSO-KCM RBF ANN, CSAPSO-FCM RBF ANN, and CSAPSO-KHM RBF ANN) for predicting the solubility of $ScCO_2$ in 4 polymers (PP, PLGA, PS and CPEs). The result is shown in Fig. 7.

The result shows that the CSAPSO-C RBF ANN model performs better than other models and it is workable to predict new experimental data under the same conditions by the CSAPSO-C RBF ANN model.

Table 1. The comparison of the test data and predicted data [43]

Tensile strength			Shear strength			Solidification temperature		
Test	**Prediction**	**Error**	**Test**	**Prediction**	**Error**	**Test**	**Prediction**	**Error**
77.47	74.89	3.22%	26.96	29.08	7.29%	184.40	187.80	1.81%
72.85	72.88	0.04%	31.84	32.41	4.94%	213.56	203.80	4.57%
77.94	75.85	2.67%	38.95	38.91	0.14%	198.83	204.80	2.92%

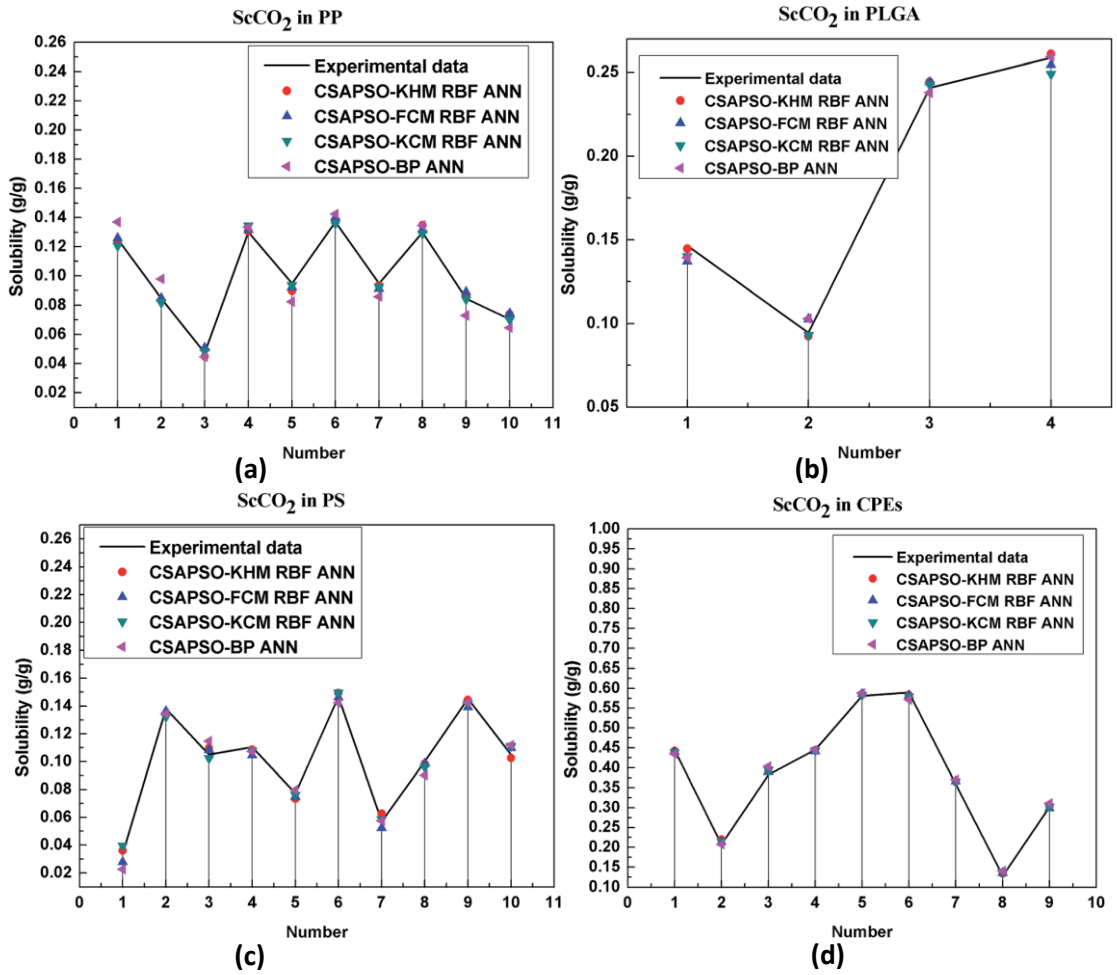

Fig. 7. Prediction of $ScCO_2$ in 4 polymers [37]

A backpropagation feed-forward neural network has been used these years because it is fast and simple to implement, and there is no need to adjust the parameters. Xie and Grossman [44] have developed a novel framework called a crystal graph convolutional neural network, which can directly extract and analyse material properties based on the connections between atoms in the crystal. The model is trained with 104 data points, and finally has achieved high accuracy in prediction. This paper advances the field of materials and provides new experiences for the design of crystalline materials.

4.2 Neural Network for the Performance Prediction of Materials

4.2.1 Fatigue life

Fatigue life is the most important parameter of fibre composites. Lee et al. [45] found it possible to model constant-stress fatigue behaviour with ANNs. For carbon-fibre composites, ANNs can produce accurate stress/R-ratio/median-life surfaces with a relatively small experimental database. The model can also be used for design, even though it is not as good at predicting minimum life as it is at predicting medium life [46].

4.2.2 Wear properties

The purpose of wear properties prediction is to perform material property, sliding agent property evaluation, and friction mechanism analysis. Jiang et al. utilized ANNs to successfully calculate the specific wear rate, frictional coefficient and some properties. To enhance the comprehensive of the analysis, 3D plots are established that showcase the predicted wear and mechanical characteristics, taking into account variations in material compositions and testing conditions. The result exhibits a strong agreement with the data, highlighting the reasonable accuracy of the methodology. Gyurova et al. [47] predicted the sliding friction

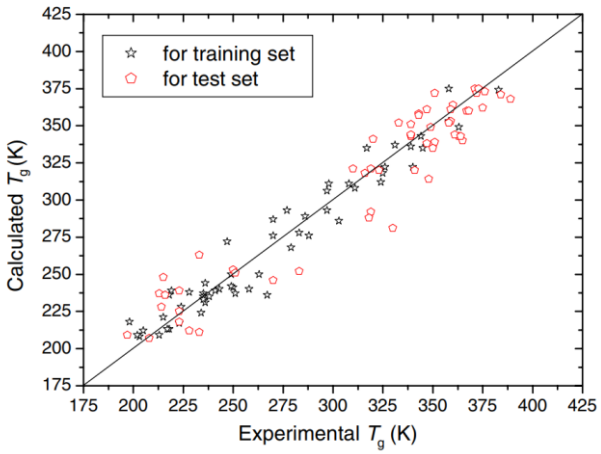

Fig. 8. Plot of experimental T_g(K) vs. calculated T_g(K)

and wear properties by 124 independent pin-on-disk sliding wear tests of polyphenylene sulfide (PPS) matrix composites and performed excellent in comparing with the measure results.

4.2.3 Thermal properties

One of the most important thermal properties of polymer composites is the glass transition temperature, T_g, which is a predecessor for predicting and understanding mechanical and other properties such as heat capacity, coefficient of thermal expansion, and viscosity. Liu et al. [48] investigates the relationship between various molecular descriptors and the glass transition temperature of polymers. To establish a predictive model, both stepwise multiple linear regression (MLR) analysis and back-propagation artificial neural network (ANN) techniques were employed. The final optimized ANN structure, consisting of 4-[4-2]$_2$-1 layer, demonstrated strong performance with a training set root mean square error (RMSE) of 11K (R=0.973) and a prediction set RMSE of 17K (R=0.955). Fig. 8 presents the comparison between experimental T_g(K) and calculated T_g(K), which shows brilliant accuracy in the prediction of glass transition temperature.

Polymer composites are excellent materials for thermal protection, which are applied in the fields of military, aircraft construction, etc. Based on BP neural network, a model of the thermal response of polymer composites without surface recession is established by Zhang et al. [41] with the purpose of improving thermal protection performance. Then they explore the relationship between bond line temperature and piecewise porosity distribution. According to the results, the approach can be well applied to the optimization of thermal protection conditions.

4.3 Neural Network for the Optimization of Materials

In an industrial process, exothermic reactive operations occur frequently. It is necessary to predict the temperature behaviour in an accurate method to avoid danger. In polymerization, specific materials are matched to specific reaction temperatures. Kuroda et al. [49] applied ANNs in modelling the behaviour of temperature in a polymerization process. The input nodes of the cooling and heating process are integrated into one node to improve accuracy and adaptability. The result shows that the model can be a useful tool for the temperature control system.

Chan et al. [50] introduces a novel approach utilizing backpropagation neural networks to model free radical polymerization in high-pressure tubular reactors. The study utilizes industrial data to train the neural network, enabling the prediction of various crucial parameters along the reactor, including the temperature profile and polymer properties. To validate the effectiveness of the neural network model, a comparison is made with predictions from mechanistic models reported in the literature. The findings demonstrate that the neural network model exhibits great promise in accurately capturing and predicting the behaviour of free radical polymerization in the reactors. This approach presents a valuable contribution to the field of polymer science and offers an alternative

to traditional mechanistic modelling techniques. Zhang focuses on the batch reactor, applying ANNs to predict the optimal control profile of the reactors. The result is much more reliable and accurate [51].

Allan et al. [52] utilized ANNs to predict the structure and properties of polypropylene fibres with key manufacturing parameters for input and fibre properties, crystal order and other parameters for output. The prediction was accurate and was able to apply in the simulation of manufacturing process.

Stephen et al. [53] employed a combination of finite element analysis (FEA) and artificial neural networks using multilayer perceptron architecture to forecast the impact resistance characteristics of hybrid and non-hybrid fabric reinforced polymer (FRP) composites. The proposed approach, combining FEA and ANNs, enables accurate prediction of the residual velocity (V_r) outcomes, thus allowing assessment of the impact behaviour of different hybrid and non-hybrid composites. The FEA and ANNs results revealed that the stacking sequence significantly influences the impact resistance of FRP composites. The highest penetration resistance was observed in specimens with Kevlar layers in the front and back (K/K/K sample).

4.4 Other Related Applications

Polyethylene as a thermoplastic has been increasingly popular in many fields. Due to the excellent performance of Ziegler-Natta catalysts in producing polyolefin with a wide range of molecular weights and copolymer compositions, researchers have employed this type of catalyst in simulating the polymerization process. The EIX (ethylene index) is the key to the process. Since it is difficult to measure the EIX, Maleki et al. [54] introduced ANNs to calculate and predict the EIX. The estimation task was carried out using the Multi-Layer Perceptron, Radial Basis, Cascade Feed-forward, and Generalized Regression Neural Networks. The results clearly indicated that the Multi-Layer Perceptron model outperformed other artificial neural network (ANN) models in terms of performance.

Rabiej et al. [55] utilized an artificial neural network that is designed to identify a specific polymer based on its Wide-angle X-ray Diffraction (WAXD) curve. The identification process involves comparing the unknown polymer's diffraction curve to a database of standard WAXD curves. The identification of the unknown polymer entails comparing the total activation signals calculated for each standard curve in the database with those calculated for the WAXD curve of the polymer. The standard curve with the highest degree of similarity to the investigated curve is chosen based on the total activation signals.

Dubdub et al. [56] presents the catalytic pyrolysis of a constant-composition mixture of zeolite β and polyethylene terephthalate (PET) polymer using thermogravimetric analysis (TGA) at varying heating rates. An artificial neural network was utilized to predict the remaining weight fraction, using temperature and heating rate as input variables. The results demonstrated that the ANN was able to accurately predict the experimental values ($R^2 > 0.999$), even when provided with new data.

4.5 Summary

This chapter focuses on the review of typical applications of artificial neural networks in polymer composites. ANNs require a large amount of data as support to accurately predict the desired parameters and the accurate *input* and *output*.

Current application cases of neural networks in polymerization are presented in terms of material design, performance prediction, and process structure optimization, respectively. By training a neural network model with the data of polymer structures and corresponding properties, it is possible to accurately predict the properties of new polymers, which reduces the trial-and-error process in polymer design. In addition, neural networks have been utilized in the field of polymer characterization. This enhances the development of high-performance polymer materials. Furthermore, neural networks have shown great potential in the prediction of polymer stability and degradation behaviour. By analysing the chemical structure and environmental factors, these networks can predict the degradation rate and lifetime of polymers.

5. CONCLUSION AND PROSPECT

Artificial neural networks have emerged as a powerful tool in the field of polymer research. These networks, inspired by the structure and functioning of the human brain, have been extensively used for various applications related to polymers. Overall, artificial neural networks

have revolutionized the field of polymers by enabling accurate property prediction, optimizing polymerization processes, interpreting characterization data, and predicting stability and degradation behaviour. As these networks continue to advance, they hold tremendous promise for further advancements in the design and development of novel polymer composites.

Several challenges that need to be addressed for the successful application of neural networks in the field of polymers. First, acquiring and processing the necessary data is of utmost importance. Polymer materials possess complex structures and diverse properties. It is necessary to get a vast amount of experimental and simulation data to effectively train neural network models. Furthermore, the accuracy and reliability of the data are critical in ensuring the overall accuracy and reliability of the trained models. Another challenge lies in improving the explanatory power of neural network models. The models are often considered *black boxes*, lacking the ability to provide specific explanations. This limitation hampers the understanding of the underlying mechanisms and undermines the interpretability of the models. Therefore, it is crucial to explore methods and techniques that enhance the interpretability of neural network models to better comprehend the relationships between polymer structure, properties, and performance. Addressing these challenges requires a lot of efforts combining polymer science, materials engineering, and data analysis techniques. Additionally, exploring techniques such as interpretability algorithms and visualization tools specific to polymer systems can aid in extracting meaningful insights from the neural network models and providing relevant explanations for their predictions.

Taking these things into account, these advancements will contribute to the development of more accurate and interpretable neural network models, facilitating the progress of polymer research and applications. By combining experimental and simulation tools, neural networks can accelerate the development of materials and encourage the various applications of polymer materials. We are looking forward to the further application and development of neural networks in polymers.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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