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Machine learning for mechanics prediction of 2D MXene-based aerogels

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ABSTRACT

Hybrid aerogels of two-dimensional (2D) transition metal carbide (MXene) and nanocellulose show huge potential in a wide range of applications owing to their unique compressive mechanical properties. However, the compressive mechanical properties of hybrid aerogels are sensitive to the physical parameters of its building blocks, which are difficult to be optimized by high throughput experiments. Considering the inherent complex variables of MXene/nanocellulose aerogels, this work realizes the prediction of their mechanical properties by machine learning (ML). Based on the reported 34 sets of data on Ti_3C_2 MXene, we trained three ML algorithms: artificial neural network (ANN), support vector machine (SVM) and random forest (RF). Results indicate that the ANN outperforms other algorithms as it fits various nonlinear input features well. The relative content of Ti_3C_2 is the most effective factor in the compressive strength of hybrid aerogel. The mechanical properties of the 540 input possibilities are predicted by the outperforming ANN model, and quantitative structural adjustment is obtained for a maximum compression modulus of 29 kPa. This work provides guideline for the mechanical property prediction of composite materials using ML.

1. Introduction

Polymer aerogels have the advantages of light weight, convenient microstructure design, variable porosity. They can be further combined with other nanomaterials that have excellent mechanical, electrical and thermal properties to synthesize multifunctional composite aerogels [1,2]. Two-dimensional (2D) transition metal carbides (MXenes) are emerging nanomaterials [3,4], which show widespread application prospects in energy storage [5], electromagnetic interference shielding [6], catalysis [7], and wearable devices [8,9]. The most-studied MXene material so far is $Ti_3C_2T_x$. $Ti_3C_2T_x$ nanosheets could be the material choice for next-generation flexible electronic devices [10], gas sensors [11], and micro- and nanoelectromechanical devices (MEMSs and NEMSs) [12]. However, the mechanical properties of the macroscopic films assembled from MXene nanosheets are relatively poor due to the interlayer strong van der Waals interactions can easily reaggregate and pile up the 2D nanosheets [13]. MXene can be assembled into macroscopic high-performance MXene-based nanocomposites through various interfacial interactions. For example, various polymers or nanomaterials containing oxygen polar groups enhance the mechanical properties of MXene sheets through hydrogen bonding [14–16]. In this regard, hybrid aerogels generated by assembling monolayer MXene nanosheets are of particular interest [17,18]. Nanocellulose aerogels tend to exhibit good mechanical properties under external forces, including compressive strength, Young's modulus and flexibility, due to the high strength of nanocellulose and the stable porous structure of the formed aerogels [19]. MXene/nanocellulose hybrid aerogel utilizes the abundant polar surface groups in monolayer MXene nanosheets to produce cross-linking effect with nanocellulose and then form a 3D porous structure aerogel with enhanced mechanical strength [20,21]. MXene/nanocellulose hybrid aerogel has the characteristics of high mechanical strength, light weight, and excellent structural stability [22].

Currently, most of the MXene/nanocellulose hybrid aerogels show compressive mechanical modulus of around 2.5 kPa, which is difficult to meet the practical applications. In order to make them more applicable, their compressive mechanical strength needs to be further improved.

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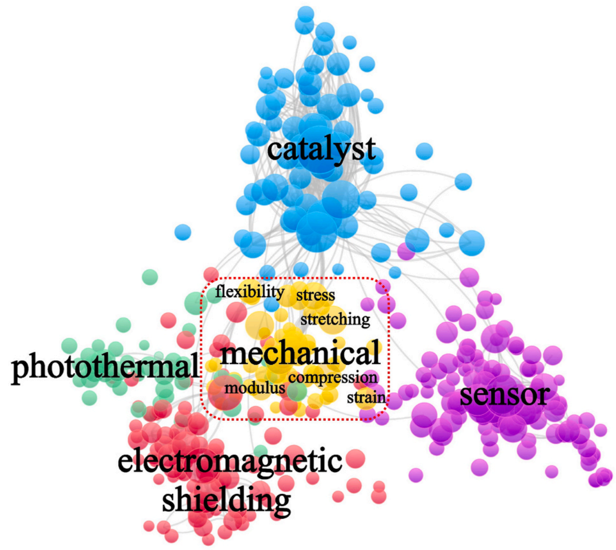

Fig. 1. Literature study of 300 papers containing keywords related to MXene aerogel. The lines between two keywords, size of circle indicate their correlations, and the frequency of key words appearance. Data were collected from web of science.

However, experimental studies on the mechanical properties of MXene/nanocellulose hybrid aerogel are still insufficient and the progress is slow compared to other applications (e.g., catalyst, sensor, photothermal, and electromagnetic shielding) as evidenced by the network co-occurring from ~300 research papers (Fig. 1). This is because the compressive mechanical properties of hybrid aerogels are sensitive to the physical parameters of its building blocks, and the slight change of any variable will cause the difference in the properties. The experimental study can only focus on the effects of few input variables and lacks empirical or semi-empirical guideline for the design and fabrication processes. Therefore, it is impossible to explore the effects of changes in various variables on mechanical properties through high-throughput parallel experimental studies.

Machine learning (ML) is used in the Material Genome Initiative (MGI) to accelerate material design by entering materials into a database [23]. The emergence of ML technology allows to explore the effect of multiple variables on the mechanical strength of MXene/nanocellulose aerogel, which can achieve results that are impossible in high-throughput parallel experiments [24]. By using ML models to train existing experimental data, the prediction results can be used to guide the design and fabrication of aerogels [25]. For example, Babak and Ahmad proposed ML-based models for predicting the thermal conductivities of polyurethane aerogel and silica–resorcinol formaldehyde aerogels [26]. Omid et al. proposed an ANN model to predict various material properties of polyimide organic aerogel through understanding the contribution materials and process factors in its synthesis [27]. The training of artificial neural network is shown in Fig. 2. The model parameters are updated by backpropagating the gradient of loss values between output and label to complete the model training process. Although ML has been used in many fields [28–30], the application in engineering science is still in infancy and is a new exploration in studying the mechanical properties of composite materials.

In this work, we plan to utilize the data reported in literatures to

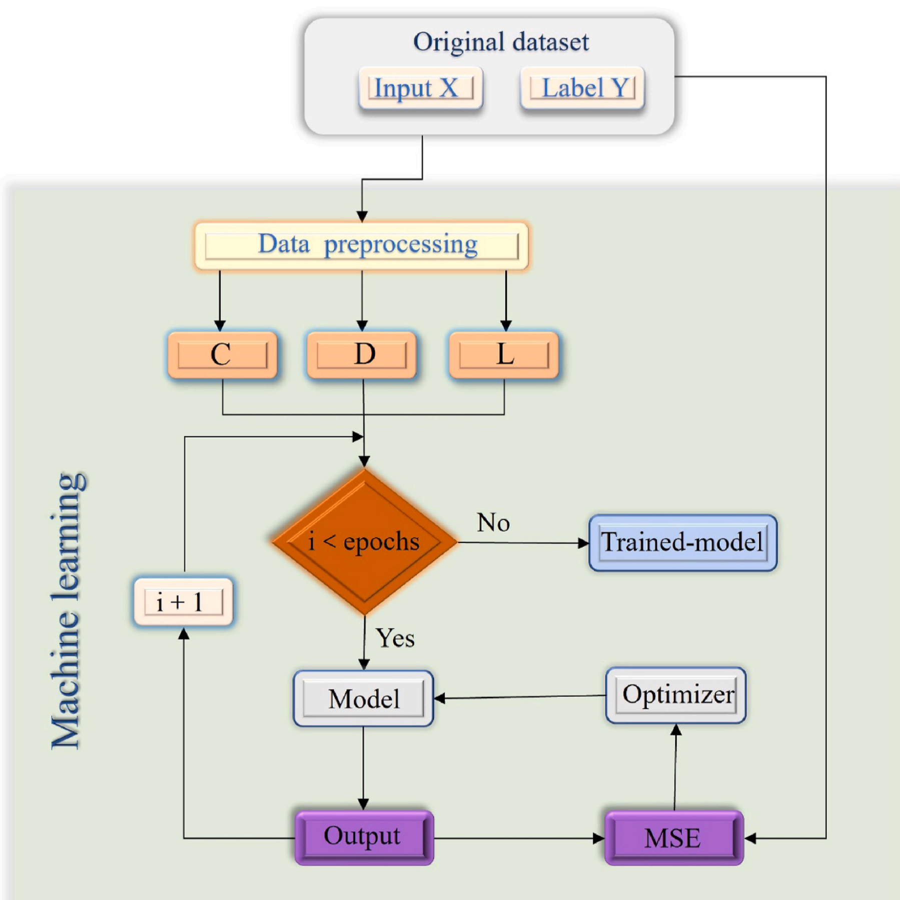

Fig. 2. Flowchart of the machine learning prediction used in this study.

Table 1
Feature description of training and testing data collected from the literatures.

Sample name	$Ti_3C_2T_x$ content (wt%)	Average diameter of carbon fiber (nm)	Average length of carbon fiber (μm)	Compression modulus (kPa)	Ref.
$Ti_3C_2T_x$	100	/	/	0.6	
$Ti_3C_2T_x$/ CNF[a]	83	1.4	0.45	1.167	[18]
	75	1.4	0.45	1	
	67	1.4	0.45	0.78	
	50	1.4	0.45	2	
$Ti_3C_2T_x$/ CMC[b]	13.04	3500	550	62.5	[34]
$Ti_3C_2T_x$/ HEC[c]	75	200	20	200	[22]
	80	200	20	153.85	
	85	200	20	166.67	
	90	200	20	136.36	
	95	200	20	90.91	
$Ti_3C_2T_x$/ CNF	10	5	0.5	31.75	[35]
CNF	0	10	1	18	
$Ti_3C_2T_x$/ CNF	25	10	1	27.5	[36]
	50	10	1	21.25	
	75	10	1	9	
$Ti_3C_2T_x$/ f-NCC[d]	25	50	0.4	15.38	[37]
$Ti_3C_2T_x$/ CNC[e]	0.4	50	0.4	2.25	[38]
$Ti_3C_2T_x$/ BC[f]	9.1	50	15	1.43	[39]
	16.7	50	15	4.62	
	33.3	50	15	4.5	
	50	50	15	3.2	
$Ti_3C_2T_x$/ MC[g]	33.3	18	0.2	214.29	
$Ti_3C_2T_x$/ MFC[h]	33.3	8000	100	6.43	
$Ti_3C_2T_x$/ CNC	33.3	50	0.4	5.22	
$Ti_3C_2T_x$/ CNF	33.3	5	0.5	4.5	
ANFs	0	30	1.5	266.67	
$Ti_3C_2T_x$/ ANFs[i]	7	30	1.5	352.94	[40]
	14	30	1.5	666.67	
	21	30	1.5	600	
$Ti_3C_2T_x$	100	/	/	0.0059	
$Ti_3C_2T_x$/ CNTs[j]	50	12	18	0.23	[41]
	33.3	12	18	0.46	
	25	12	18	0.57	

[a] CNF refers to cellulose nanofibril.
[b] CMC refers to carboxymethyl cellulose.
[c] HEC refers to hydroxyethyl cellulose.
[d] f-NCC refers to functionalized cellulose nanocrystal.
[e] CNC refers to cellulose nanocrystal.
[f] BC refers to bacterial cellulose fiber.
[g] MC refers to methylcellulose.
[h] MFC refers to microfiber cellulose.
[i] ANFs refers to aramid nanofibers.
[j] CNTs refers to carbon nanotube.

predict the compressive mechanical properties of hybrid aerogel using different ML algorithms. The relationship between the composition and mechanical properties of hybrid aerogels will be quantitatively analyzed through ML. Finally, we will systematically study the mechanisms affecting the mechanical properties of MXene/nanocellulose hybrid aerogels in terms of different material composition variables (the relative content of MXene nanosheets and carbon fibers size).

2. Data and methodology

We normalized the variables affecting the mechanical properties from the composition of the hybrid aerogel, and the relative content of MXene and the diameter and length of carbon fibers were used as three input variables for prediction. Noted that the hybrid aerogel needs to undergo heat treatment and carbonization to get the final sample, which is essentially a mixture of MXene and carbon fibers [31]. In this section, we will describe the collection of data affecting the mechanical properties of the hybrid aerogel, the cleaning and preprocessing of the data, and the ML algorithm used in this work.

2.1. Data collection and preprocessing

In order to build a neural network model, the first stage is to collect relevant and representative data, which are derived from the literatures and existing databases. The size of the collected dataset largely depend on the amount of literature accumulated in the field [32]. $Ti_3C_2T_x$ is the first MXene material to be discovered and the most extensively studied to date [33]. Monolayer $Ti_3C_2T_x$ can already be produced in large quantities, which is the mostly used MXene in hybrid aerogels. Therefore, this work focuses on $Ti_3C_2T_x$-based aerogels. To create a more accurate model, these data need to cover three variables that affect the mechanical properties of the $Ti_3C_2T_x$/nanocellulose hybrid aerogel. We collected all relevant literatures from the Web-of-Science database through keywords search and established the required dataset. The dataset contains 34 experimental samples, as shown in Table 1.

Data cleaning and preprocessing are key steps in building more accurate prediction through ML [42]. The collected 34 sets of data cannot be directly used in the original format, which need to be manually checked for errors, missing or inconsistent points (outliers). By normalizing and standardizing the data, excessive values should be removed, and all the variable values can be specified within a certain value range (Table S1), which improves the prediction performance of ML model.

2.2. Machine learning algorithms training

Through a large number of calculations, ML can find the relationship between data more easily than human beings, and then establish a network to connect these relationships. In recent years, ML has been widely used in materials science [43–45] and mechanics [46–48] to reveal the relationships between various parameters of materials and their effects on mechanical properties. In order to study the influence of carbon fiber size on the mechanical properties of aerogels, we choose supervised ML algorithm to use the collected data for regression analysis and realize the prediction of the mechanical properties of aerogels. Common regression algorithms including support vector machine (SVM), random forest, gradient boosting machine (GBM), artificial neural network (ANN) and so on. SVM maps input data into high-dimensional space by selecting different kernel functions and optimizes the model by adjusting regularization parameter (C) and gamma (kernel coefficients). Random forest is an algorithm based on decision tree, which adjusts the model by adjusting the number of decision trees and the number of features to be considered in splitting. GBM combines multiple decision trees to build a prediction model and can learn from the mistakes of the previous decision trees, and then correct the next tree to achieve better results. ANN is an advanced ML model, which can imitate the learning process of human brain and establish a large number of connected neurons through a series of weight parameters [49–51]. The process of training is to optimize the value of these weight parameters so that the model can get better results [52]. Adjusting the numbers of hidden layers and neurons in each hidden layer is an important method for optimizing the ANN model.

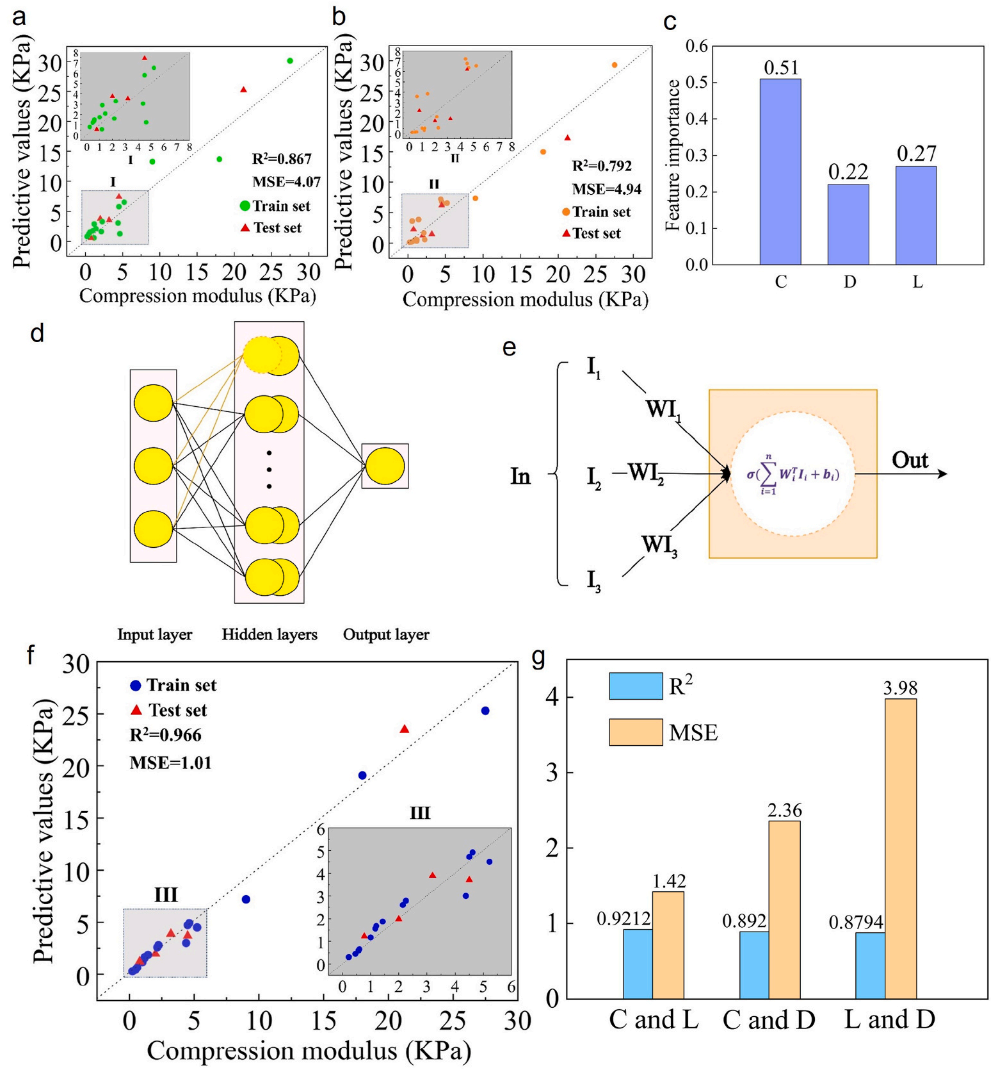

Fig. 3. Predictive values of SVM, Random forests and ANN machine learning models. (a) Predictive values of SVM model. (b) Predictive values of random forest model. (c) Importance of input characteristics obtained from random forest model. (d) Network structure of artificial neural network. (e) Individual neurons in the hidden layer. (f) Predictive values of artificial neural network mode. (g) Model performance trained by randomly selecting two different parameters as model inputs. C, D and L represent $Ti_3C_2T_x$ content, average carbon fiber diameter and average carbon fiber length respectively.

3. Result and discussion

In this work, we divided the total data set into training set and test set according to the proportion of 4:1. We used the training set to train three different models to predict the mechanical properties of MXene/nanocellulose hybrid aerogels, and used the test set to verify the models. Firstly, we train a SVM model. SVM maps non-linear data to the high-dimensional space to make non-linear data linearly separable in high-dimensional space through kernel function. Converting the regression problem into a set of linear equations for solution leads to faster training process and better accuracy [53]. We used Gaussian kernel function to build a SVM regression model and predict the mechanical properties of aerogels. The results are shown in the Fig. 3a. The R^2 score of the model is 0.867, and the mean-square error (MSE) is 4.07. These results can preliminarily determine that there is a strong correlation between input and output. To explore the priority of the three input characteristics, we trained a random forest regression model. Random forests predicted the mechanical properties of aerogels by constructing different training sets to train multiple decision trees and then calculating the average output value of all decision trees [54]. Due to the discontinuity of the output of the regression decision tree, this model is usually used in the case of low precision requirements. The prediction results of Random forests model are shown in the Fig. 3b. The R^2 score and MSE of the model are 0.79 and 4.94 respectively. In addition, the random forest model can also obtain the importance of each input feature according to the importance of different leaf nodes (Fig. 3c). The importance of $Ti_3C_2T_x$ content, average carbon fiber diameter and average carbon fiber length is 0.51, 0.22, 0.27 respectively.

To verify the feature importance results obtained from the RF model and improve the prediction accuracy of the mechanical properties of hybrid aerogel, we trained an ANN model to improve the prediction accuracy of the mechanical properties of hybrid aerogel (Fig. 3d-e). The ANN model includes an input layer and an output layer and three hidden layers. Each hidden layer contains six neurons. Layers are activated by Sigmoid function and trained with a learning rate of 0.005. The input features are transferred to the hidden layer neurons through a set of weight parameters, and then the hidden layer neurons get the output of the model through nonlinear transformation and feature transfer. The results of the model are shown in Fig. 3f. ANN model fine regulates the relationship between each neuron, by virtue of multiple nonlinear layers and a large number of weight parameters, so that ANN can well adapt to various nonlinear input features. Therefore, the performance of ANN model is better than that of SVM model and random forest model.

In order to explore the importance of different features, we also selected two different features as the input of the artificial neural network for training. The results are shown in Fig. 3g. It can be found that when $Ti_3C_2T_x$ content and average carbon fibers length are used as inputs, the model performance is better than the other two cases. This result matches the feature importance given by the random forest mode.

By analyzing the data in the literatures, we found that the ranges of

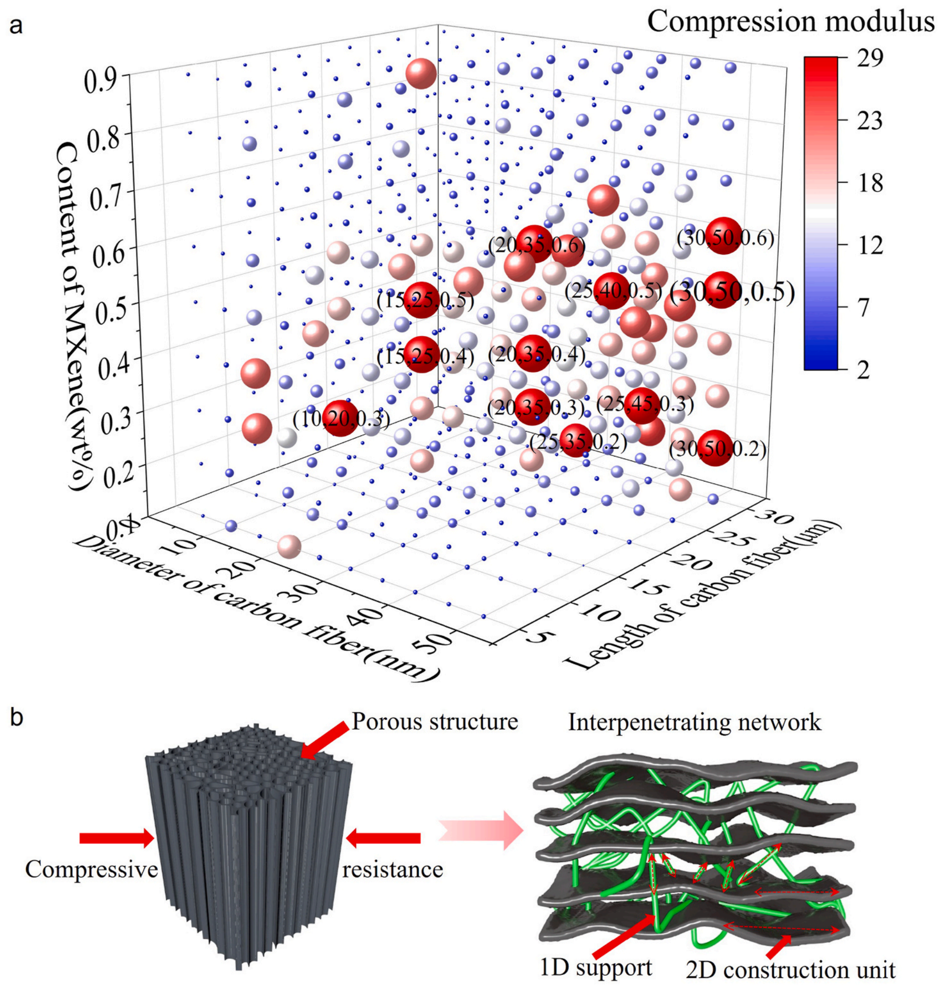

Fig. 4. Mechanical properties predicted by ANN machine learning models, and the structure of MXene/nanocellulose hybrid aerogels composition. (a) Mechanical properties of hybrid aerogels under different input parameter combinations predicted by the model, the size of the spheres represents the magnitude of the compression modulus. (b) Schematic illustration of 1D/2D interpenetrating network of MXene/nanocellulose hybrid aerogels.

three key parameters: content of MXene 0.1–0.83, diameter of carbon fibers 1.4–50 nm, and length of carbon fibers 0.5–27.5 μm. We took nine points equally spaced in the content of MXene range, ten points in the diameter of carbon fibers range, and six points in the length of carbon fibers, and then combined these points into 540 input possibilities. Then we predicted the mechanical properties of these 540 input possibilities on the best performing ANN model, and the results are shown in Fig. 4a. The predicted mechanical properties of the model reached the maximum 29 kPa under the combination of (30, 50, 0.5). The number of 30, 50, and 0.5 representing the length of carbon fibers, diameter of carbon fibers, and content of MXene, respectively. The model also predicted high mechanical performance in combination of (30, 50, 0.6), (20, 35, 0.6), (20, 35, 0.3), and so on (the 11 big red spheres in Fig. 4a), which all reached compressive mechanical properties above 26 kPa. Researchers can refer to these results to design parameters of hybrid aerogels near these red balls to obtain greater mechanical properties.

Next, we specifically discussed the effects of different variables on the mechanical properties of MXene/nanocellulose hybrid aerogels from the view of composition. $Ti_3C_2T_x$ nanosheets have abundant functional groups on the surface, which can easily cross-link with nanocellulose to form strong hydrogen bonds [34]. Such hydrogen bonds make them form continuous, oriented and wavy-like lamellae, which increases the connection strength between $Ti_3C_2T_x$ nanosheets and the structural stability of hybrid aerogel [18]. Their horizontal dimensions can reach several square microns and have excellent mechanical strength (Young's modulus of 333 ± 30 GPa for monolayer nanosheets) [55]. In brief, $Ti_3C_2T_x$ nanosheets act as "bricks" in $Ti_3C_2T_x$/nanocellulose hybrid aerogel, and cellulose as "mortar" can improve the gelation between nanosheets. If the relative content of $Ti_3C_2T_x$ is too low, the nanosheets are not enough to provide sufficient stiffness and strength. Conversely, if the relative content of $Ti_3C_2T_x$ is too high, the stacking of nanosheets will occur. The results in Fig. 4a show that compressive mechanical properties are higher when content of $Ti_3C_2T_x$ is 0.2–0.6. Therefore, according to the predicted results, the researchers can choose the appropriate relative content to effectively control the lamellar structure of the hybrid aerogel, so as to adjust the mechanical properties.

Nanocellulose has been used as the reinforcing linkers of MXene hybrid aerogel because of its abundant source, high mechanical strength, light weight and strong sustainability [56]. Nanocellulose has different diameters and lengths and exhibits typical rod-like morphology [57]. Nanocellulose can be embedded between MXene nanosheets. After cross-linking nanocellulose with MXene, a 1D/2D interpenetrating network was constructed (Fig. 4b), so nanocellulose has a significant supporting effect on MXene nanosheets [34]. The strong interfacial adhesion between carbon fibers and nanosheets allows stress to be transferred or distributed from nanosheets to fibers during deformation, thus improving the toughness and compression resistance of the hybrid aerogel film. In detail, repeated breakage and reformation of hydrogen bonds between adjacent interfaces and energy dissipation occur under stress [58]. The size and porosity of carbon fibers play critical roles in the deformation of hybrid aerogels. The above factors can be affected by the modification of cellulose, so as to improve the mechanical properties

[59]. In addition, a solid 3D network structure is formed, which improves the flexibility and recoverability of the hybrid aerogel. The hybrid aerogels composed of different sizes of nano-cellulose have different 3D network and porous structure, which will lead to different mechanical properties of the material [40].

4. Conclusions

In this study, machine learning models of support vector machine (SVM), random forest (RF), and artificial neural network (ANN) were used to predict the compression modulus of $Ti_3C_2T_x$/nanocellulose hybrid aerogel using data sets obtained from the literatures. The results of the three models show a high degree of consistency, which fully proves that the mechanical properties of the hybrid aerogel are highly related to the content of $Ti_3C_2T_x$ and the size of carbon fibers. In addition, from the perspective of the importance of the input features obtained from the RF model, the relative $Ti_3C_2T_x$ content was the most significant parameter affecting the mechanical properties of the hybrid aerogel (the importance reached 0.51). The training accuracy of ANN model ($R^2 = 0.966$, MSE = 1.01) are superior to SVM model ($R^2 = 0.867$, MSE = 4.07) and RF model ($R^2 = 0.792$, MSE = 4.94). Finally, we predicted the mechanical properties of hybrid aerogels under a large number of input possibilities. These results provide a reference for the material optimization and condition design of $Ti_3C_2T_x$/nanocellulose hybrid aerogel in the future.

CRediT authorship contribution statement

Chao Rong: Data curation, Writing – original draft, preparation. **Lei Zhou:** Methodology, Software, Writing – original draft, preparation. **Bowei Zhang:** Conceptualization, writing, Supervision, and, Funding acquisition. **Fu-Zhen Xuan:** Supervision.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Bowei Zhang reports financial support was provided by National Natural Science Foundation of China

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.coco.2022.101474.

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