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Prediction of mechanical properties of carbon fiber based on cross-scale FEM and machine learning

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ABSTRACT

Carbon fiber is the most common reinforcing phase in composite materials. However, it is difficult to obtain the performance parameters of the monofilament. In this study, the relationship between the property variables of the carbon fiber monofilament and the macroscopic parameters of the composites is established using a regression tree, a type of decision tree model, in machine learning. First, in order to obtain the data for machine learning, representative volume element (RVE) models of single-layer and multi-layer carbon fiber reinforced plastic (CFRP) are established by a cross-scale finite element method (FEM), and periodic boundary conditions are loaded. Then, a correlation model between the carbon fiber properties and CFRP and matrix properties is established. The non-GUI mode is called by Software Isight to generate the sample data. Second, in order to avoid overfitting, the L1 norm method is used for feature selection before model training. Finally, the four elastic properties of the carbon fiber are analyzed by a regression tree model. After a series of parameter adjustments and model selection, the model with a better generalization performance was obtained. The validity of the models was verified by the validating sample set.

1. Introduction

Carbon fiber reinforced plastic (CFRP) is a multi-phase solid material consisting of two or more materials with different physical and chemical properties, and the use of this material in aerospace systems has increased in recent years [1]. The continuous symmetry of the composites is a matrix, and the dispersed phase is the reinforcing phase. All phase materials reinforce each other, and the overall performance achieved is superior that of a single material.

As one of the most commonly used reinforcing phases of aerospace composites, the carbon fiber mechanical properties play an important role in the evaluation of the composite comprehensive properties, simulation of component deformation, and prediction of damage behavior. The engineering community utilizes the mechanical property test of the carbon fiber, and national associations or enterprises have developed relevant testing standards, such as JIS R7608-2007 (Carbon fiber – Determination of tensile properties) in Japan, ASTM D4018-2011 (Standard Test Methods for Properties of Continuous Filament Carbon and Graphite Fiber Tows) in America, and GB/T26749 in China. However, because of the carbon fiber's tiny size, high artificial effect, and high discrete value of the performance, the testing is expensive. In addition, the results are not reliable, which is a problem faced by engineers [2]. There are several engineering solutions to this problem, such as testing the carbon fiber bundle instead of the carbon fiber monofilament or increasing the sample size to exclude random factors. However, it is difficult to achieve a satisfactory balance between the accuracy and cost.

The matrix phase and reinforcing phase of the composite materials are arranged in order at the micro level to form macroscopic materials; thus, the mechanical properties have a one to one correlation. The theory of composite laminates is well established, and the macroscopic properties of the composite materials can be deduced according to the properties and arrangement of the fiber and matrix [3,4]. The theories of the laminates are based on mathematical formula that ignore the stress in the depth of the material and have special boundary conditions, creating some problems. Under the actual force or the complex surfaces, the finite element method can directly reflect the structure characteristics of the composite materials and construct the relationship between the micromechanics and macroscopic mechanics. Tang [5] proposed an analysis method based on a numerical simulation and mathematical modeling after the weaving model was established. Huang [6] proposed a versatile and easy-to-use micro composite model, which can simulate the elastic, elastoplastic, and stress limits of two-dimensional braided composites under arbitrary loads. Donadon et al.

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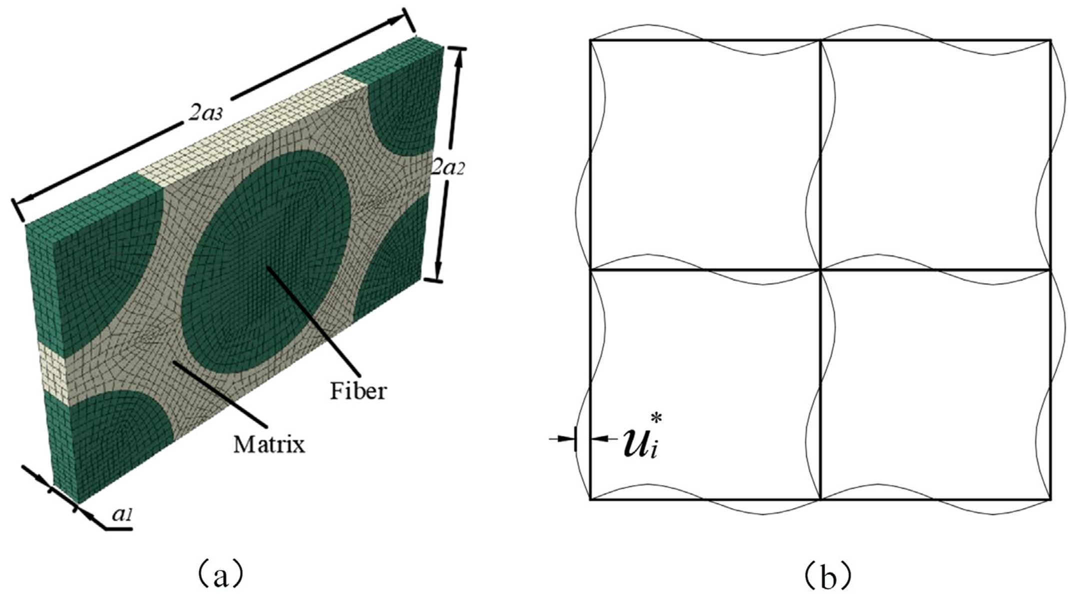

Fig. 1. RVE model and boundary conditions.

[7] presented an analytical model for the prediction of the elastic behavior of plain-weave fabric composites based on classical laminate theory, and the theoretical predictions were compared with the experimental results and predictions using alternative models available in the literature. Chun et al. [8] examined the effects of a z-pin reinforcement on the elastic properties of composite materials as well as the changes in the elastic properties based on the diameter of the z-pin. Kamiński et al. [9] proposed computational techniques based on the finite element method (FEM) solution of the cell problem to discover the sensitivities and uncertainties in the homogenized tensor that resulted from variations of the material parameters in the CFRP. Kamarudin et al. [10] established a three-dimensional finite element model of unidirectional fiber reinforced composites using a periodic boundary condition method to predict the elastic mechanical behavior of a unit cell of such composites. Yang et al. [11] numerically simulated the tensile behavior of a three dimensional (3D) orthogonal woven composite based on the unit cell model. The influence of the crack damage and the stress on the fiber, resin, and fiber/resin interface were analyzed. Sun et al. [12] developed a multi-scale computational analysis based on representative volume element modeling and molecular dynamics simulations to investigate the microscopic failure mechanisms of unidirectional CFRP composites. These representative studies predicted the properties of composite materials using a finite element method, and verified by performing experiments, which demonstrated the validity of the finite element method in building the meso-macro performance relationship of the composite material.

In practice, macro performance parameters are easy to obtain. If the microscopic parameters can be obtained by measuring macro parameters, the cost would be reduced, and the efficiency would be improved. Because of the complex nonlinear relationship between the macro and micro performance parameters, the theoretical method should solve complex transcendental equations, which is not a realistic expectation.

Therefore, machine learning is used as a reference. Machine learning is a modeling method for creating the relationship between input and output quantities from a given data set through algorithmic iteration. Given only historical data, the algorithm can generate the model automatically according to the iteration rules of the selected model. Once the model is built and tested, the model can predict the output value of the newly generated input information. A regression tree model is a machine learning method, which has low modeling and calculation costs and a high prediction accuracy [13,14]. The regression tree model has been applied in numerous fields involving data analysis, such as transit service quality analysis [15], listing status prediction of companies [16], software fault prediction [17], soil unit prediction [18], etc.

In this study, the decision tree model is applied to establish the relationship between the micro and macro properties of composite materials to achieve accurate and rapid prediction of the micro properties. First, ABAQUS software is used to established the finite element model, and sets of data for model training and testing are obtained. Then, in order to improve the generalization performance of the model, the feature selection of the original data is carried out before the model training, and dimensionality reduction of the data is realized. Finally, the decision tree model is established according to the object to be predicted, and the optimal prediction model is obtained by adjusting the parameters.

2. FEM modeling and obtaining the data set

A sufficient amount of data should be collected for model training and checking. Without considering the cost factors, experimental methods cannot meet the requirements of data diversity. Therefore, a finite element model is established to generate the property data using a representative volume element (RVE) under periodic boundary conditions. Isight software is used to organize the input data and call Software Abaqus using the noGUI mode. A detailed description of the FEM modeling is presented in a previous article [19].

2.1. FEM modeling

CFRP is composed of multiple layers of unidirectional materials. First, an RVE model of the unidirectional CFRP (UD-CFRP) should be established to predict the mechanical properties.

In order to realize modeling and solving of the materials, the composite materials should be idealized at the structural level. The composite material is assumed to be intact, and the fiber is combined with the matrix. The voids and initial micro cracks produced during fabrication are neglected, in which the fiber is transversely isotropic, and the matrix is isotropic. Because of the randomness of the fiber arrangement in the actual structure, the fiber arrangement is simplified to a uniform distribution or staggered distribution in the modeling process. Because the staggered arrangement is closer to the random distribution of the fiber, the rectangular staggered RVE is used to predict the anisotropic

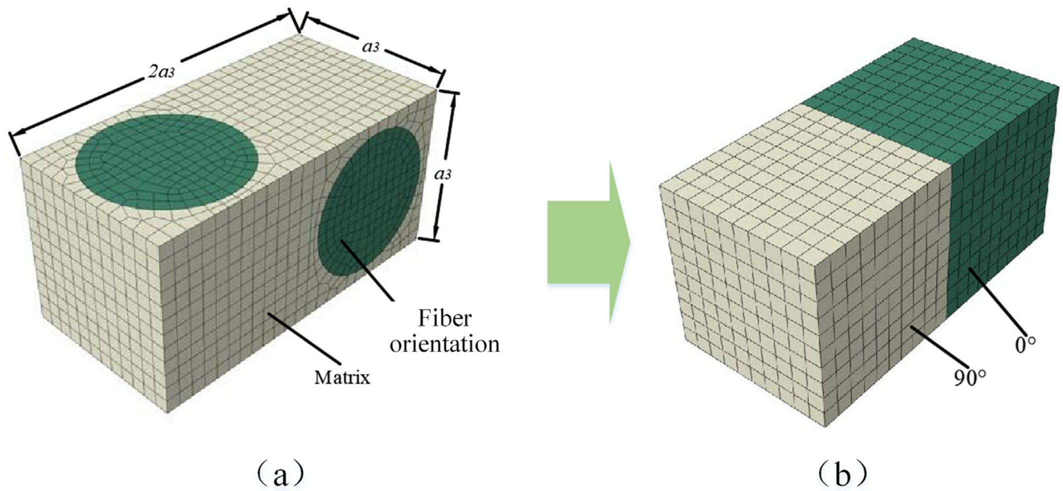

Fig. 2. RVE model and boundary conditions: (a) Fiber orientation of the [0/90°] CFRP and (b) RVE of the [0/90°] CFRP.

properties of the composites, as shown in Fig. 1(a). The dimensions in the RVE model are determined from the basic geometric parameters of the composite materials and fibers.

The elastic properties of the carbon fiber and matrix are defined in the software program. Carbon fiber is treated as a transverse isotropic material, and the elastic constants are applied to characterize the mechanical properties, including the Young's modulus, fE_1, $fE_2 = fE_3$, shear modulus, $fG_{12} = fG_{13}$, fG_{23}, Poisson's ratio, $f\nu_{12} = f\nu_{13}$, and $f\nu_{23}$. The elastic constants of the matrix are defined as an isotropic material, including the Young's modulus mE and Poisson's ratio $m\nu$.

A normal stress and shear stress of 1 MPa are applied in three directions, and the corresponding stress nephogram under each load is obtained. According to the applied load and the strain response, the predicted values of the elastic modulus and shear modulus of UD-CFRP in all directions can be calculated, including the Young's modulus, $E_1 = E_2$, E_3, shear modulus, G_{12}, $G_{13} = G_{23}$, Poisson's ratio, ν_{12}, and $\nu_{13} = \nu_{23}$.

For multidirectional CFRP (MD-CFRP), one single layer could be considered a UD-CFRP. With [0/90°] CFRP, the RVE could be established considering the different fiber orientation, as shown in Fig. 2. The RVE is combined by two parts with different mechanical properties, which are obtained from the calculation of the UD-CFRP.

Similar to the UD-CFRP, a normal stress and shear stress of 1 MPa are applied in three directions, and the corresponding stress nephogram under each load is obtained. The values of the elastic modulus and shear modulus of the UD-CFRP in all directions can be obtained.

2.2. Obtaining the data set

The effectiveness of machine learning is dependent on the large amounts of data sets, which contain a training sample and checking sample. Since one sample can be obtained for each FEM model, it is time consuming to obtain all samples individually. Isight software is used to organize the input data that is generated using the Monte Carlo method. The FEM modeling step is recorded to generate the PY file with parameterized codes. The PY file could be called by Isight and run in non-GUI mode, which will improve the computational efficiency.

Five hundred samples were prepared for model training and checking. Several samples are listed as examples in Table 1. Since the Poisson's ratios could be calculated through the Young's modulus and shear modulus, they were deleted from the sample and were not treated as valid features.

3. Feature selection based on L1 norm

Given a data set, each of the attributes are referred to as features, such as the elastic modulus of the fiber, Poisson's ratio of the matrix, etc. Feature selection is the process of selecting the feature subset with the greatest correlation to the output data from the feature set of the sample [20]. Feature selection is an important step in data processing. Its purpose is to select the feature subset that has the greatest relevance to the current learning task from all feature sets, simplify the model, decrease the computational cost of the model, and reduce the risk of over-fitting.

3.1. The process of feature selection

Feature selection is generally divided into two steps. The first step is a subset search, and the second step is a subset evaluation. An embedded selection is a selection method that combines feature selection with the learning process. As one method of embedded selection, the L1 regularization algorithm can easily obtain a sparse solution to achieve feature selection. This method considers the data set and learning tasks and avoids a large computation; therefore, it is applied for feature selection in this study.

The purpose of this study is to predict the fiber performance parameters; thus, the features listed in Table 1 should be recognized. The elastic parameters of the CFRP and matrix are defined as the input data, labeled F0–F5. The fiber elastic parameters are the output data labeled F6–F9, as listed in Table 2.

The program of feature selection is written in Python according to the flow chart shown in Fig. 3.

3.2. Feature selection of the output data

Feature selection of the fiber longitudinal elastic modulus fE_1 is carried out, and the weight ratio is shown in Fig. 4. Feature 0, the elastic modulus of CFRP E_1 ($E_2 = E_1$), has a significant effect on fE_1, while the other feature effects are nearly negligible. This is consistent with results of the previous studies. The elastic properties of the fibers determine the properties of the CFRP in the fiber orientation and vice versa.

Feature selection of the fiber transverse elastic modulus fE_2 ($fE_3 = fE_2$) is carried out, and the weight ratio is shown in Fig. 5. This situation is different from that in Fig. 4. Features 1 and 4, the elastic modulus of CFRP E_3 and elastic modulus of matrix mE, have a significant effect on fE_2, while the other feature effects are individually smaller; however, the effects cannot be ignored.

Table 1
Several samples of the data set (GPa).

No	Fiber			Matrix				CFRP		
	fE_1	fE_2/fE_3	fG_{12}/fG_{13}	fG_{23}	mE	$m\nu$	E_1/E_2	E_3	G_{12}	G_{23}/G_{13}
1	155183.9	5676.46	16719.06	13699.34	1694.076	0.174561	48.28472	3.498697	2.659311	2.120019
2	240807.7	18162.21	18859.44	7793.484	3640.422	0.366412	77.82365	10.53344	4.465141	3.439052
3	168299.4	12334.73	24852.19	3024.314	1444.104	0.192185	52.66667	4.13852	2.398585	1.585691
4	193,953	13790.01	11116.56	8518.753	3390.328	0.383944	62.88932	9.420868	3.641958	3.103078
5	132242.7	17159.39	23656.16	11831.93	2807.759	0.216146	43.75523	7.199494	4.169607	3.234731
6	233,628	7148.917	12312.97	6362.479	4861.649	0.281865	73.84071	6.914798	5.0241	3.997205
7	186,861	18007.66	16231.13	7607.108	4208.89	0.334704	61.97462	10.66212	4.866547	3.804595

Table 2
Number of the features.

F0	F1	F2	F3	F4	F5	F6	F7	F8	F9
E_1/E_2	E_3	G_{12}	G_{23}/G_{13}	mE	$m\nu$	fE_1	fE_2/fE_3	fG_{12}/fG_{13}	fG_{23}
CFRP				Matrix		Fiber			
Input data						Output data			

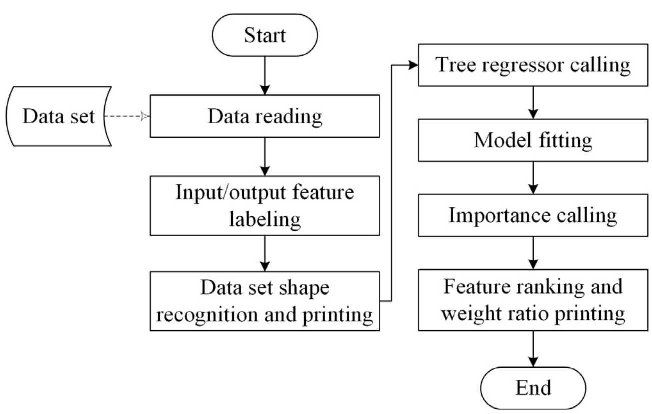

Fig. 3. Flow chart of feature selection.

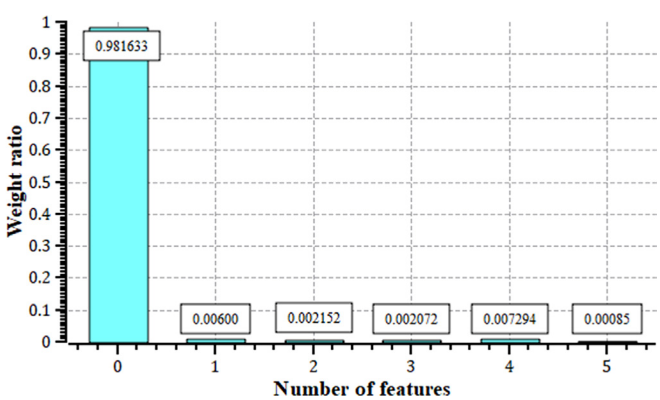

Fig. 4. Weight ratio of fE_1.

Feature selection of the fiber shear modulus fG_{12} ($fG_{13} = fG_{12}$) is carried out, and the weight ratio is shown in Fig. 6. The situation is similar to that in Fig. 5. Features 2 and 4, the shear modulus of CFRP G_{12} and elastic modulus of matrix mE, have a significant effect on fG_{12}, while the other feature effects are individually smaller; however, the effects cannot be ignored.

Feature selection of the fiber shear modulus fG_{23} is carried out, and the weight ratio is shown in Fig. 7. The four features have a significant effect on fG_{23}; features 2, 3, 4, and 5; the shear modulus of CFRP G_{12} and G_{23}; and the elastic modulus and Poisson's ratio of the matrix mE and $m\nu$.

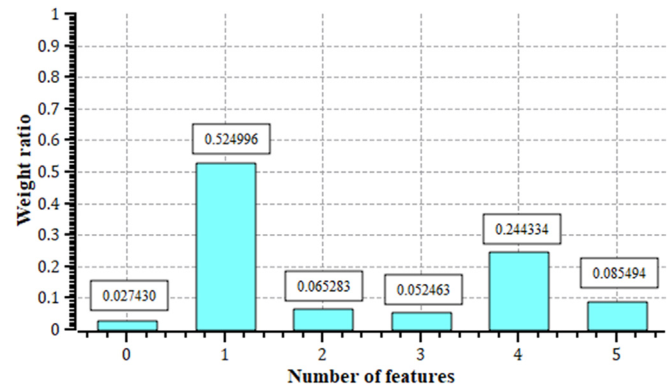

Fig. 5. Weight ratio of fE_2.

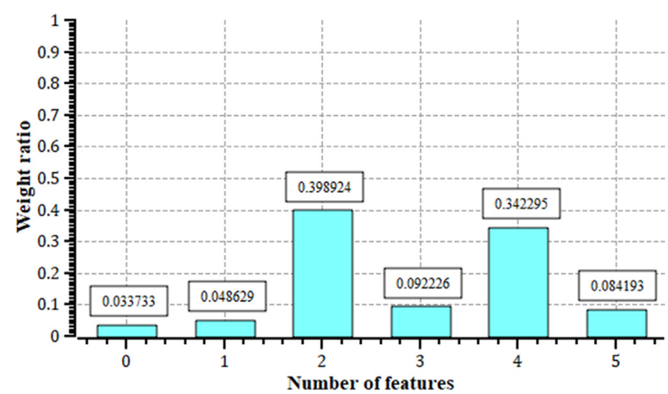

Fig. 6. Weight ratio of fG_{12}.

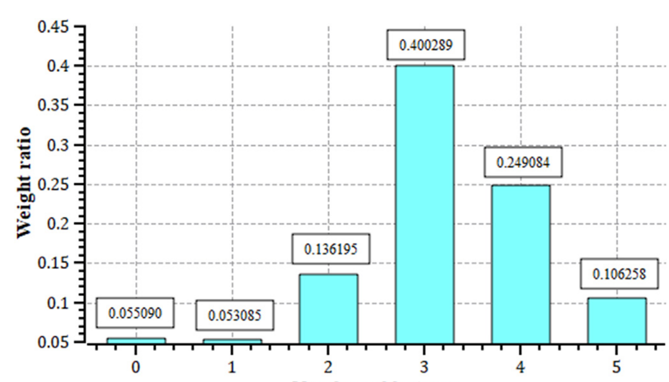

Fig. 7. Weight ratio of fG_{23}.

The correlation of the features could be obtained through the correlation coefficient calculation. A global reflection of the correlation of all the features is shown in Fig. 8

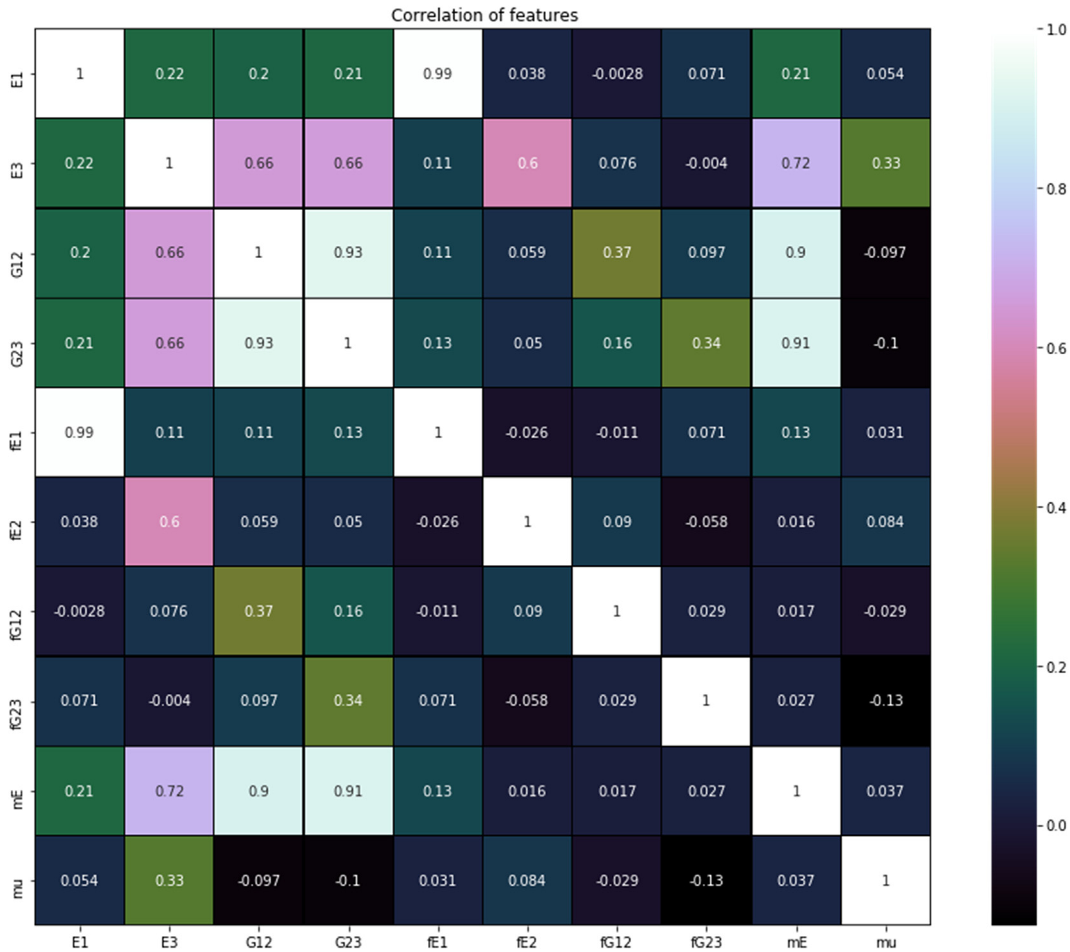

Fig. 8. Correlation of the features.

4. Property prediction based on decision tree regression

The decision tree model can realize data classification and regression, such as decision tree classification and decision tree regression. In this study, the decision tree regression algorithm classification and regression tree (CART) is used, which was derived from the algorithm proposed by Breiman et al. [21]. The learning process includes the following steps:

(1) Divide all the data into a training set and test set.
(2) Generate a regression tree model to fit the training set data.
(3) Predict the output value of the test set data with the learning model.
(4) Compare the predicted value of the model with the true value of the test set. The predicted root mean square error and error rate are obtained.
(5) Determine the two curves of the predicted value and the real value of the model using the serial number of the test data as the horizontal axis and the output value as the vertical axis, respectively.

The model depth represents the complexity of the model; thus, selecting the optimal model selects the optimal tree depth. The depth of the tree could be adjusted. When the tree is deeper, the model more precisely describes the details of the training set. However, a tree that is too deep will cause over-fitting. Therefore, in order to obtain an appropriate model, experiments are carried out on model trees with multiple depths.

Because the training data set is small, and the probability of over-fitting is high, the ideal model can be obtained by setting a small tree depth and adjusting the random seed number.

4.1. Prediction of the longitudinal elastic modulus fE_1

According to the above decision tree training and prediction process, the prediction results of the tree depths of 2, 3, 4, and 5 are shown in Fig. 9. The acronym RMSE represents the root mean square error between the predicted value and actual value. The term AV represents the average of the actual value. Thus, RMSE/AV is a ratio that shows the overall deviation degree of the predicted sample. The rate of the error is the ratio of the predicted error sample to the total number of samples, and the smaller the rate, the better the prediction accuracy. However, a model with a small error rate may also have a risk of over-fitting; therefore, a variety of factors should be selected.

For the prediction results of fE_1, the accuracy of the model was satisfactory. When the tree depth increased to 3, the error rate and RMSE/AV decreased. As the tree depth increased further, the reduction of the error rate and RSEM were not significant; therefore, the decision tree model with a tree depth of 3 was selected for the fE_1 prediction.

4.2. Prediction of the transverse elastic modulus fE_2/fE_3

Similar to the prediction process of fE_1, the prediction results of the tree depths of 5, 6, 7, and 8 are shown in Fig. 10. When the tree depth increased to 7, the error rate and RMSE/AV decreased. As the tree depth increased further, the error rate and RSEM increased. This probability was from over-fitting. Therefore, the decision tree model with a tree depth of 7 was selected for the fE_2/fE_3 prediction.

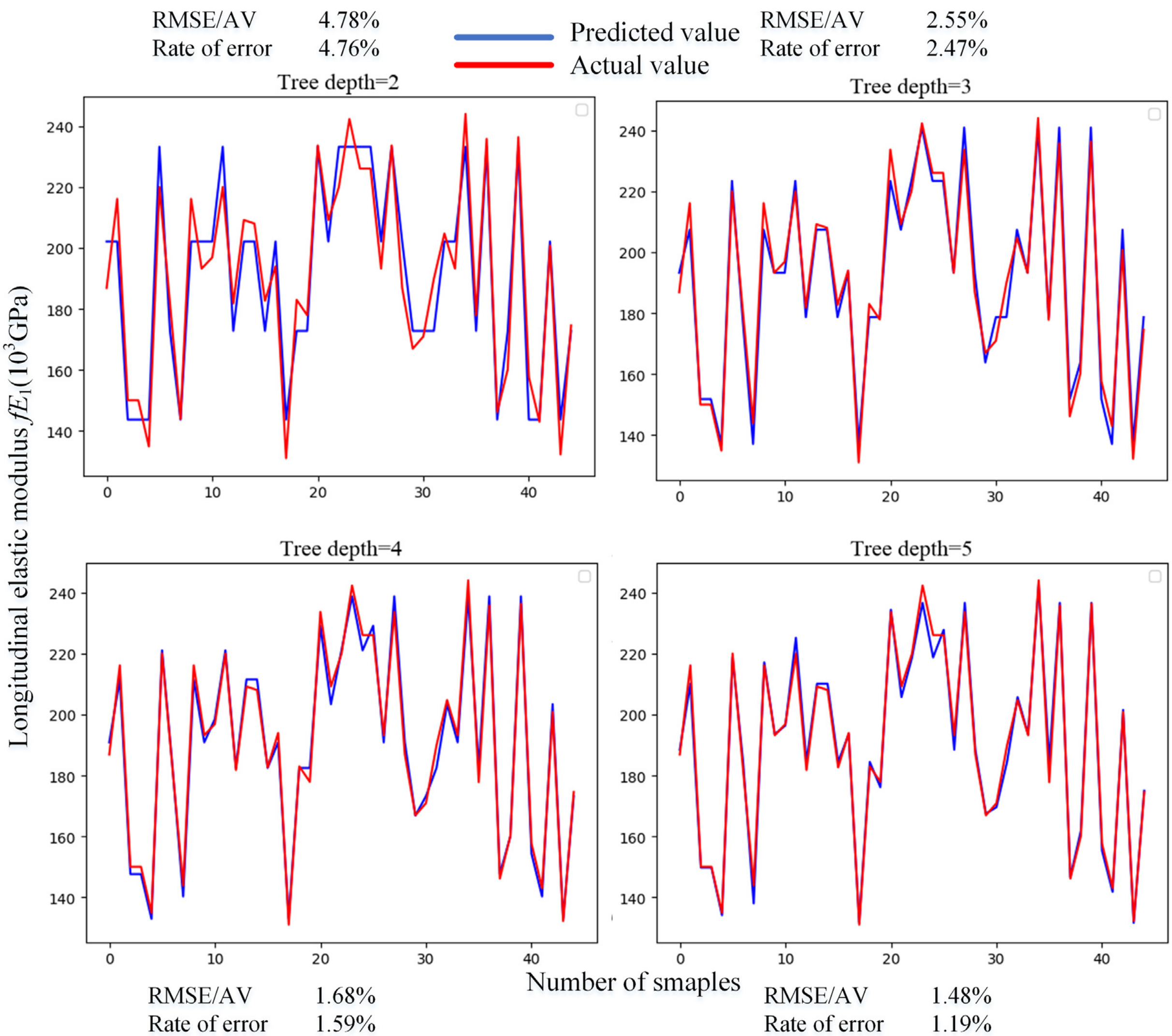

Fig. 9. Prediction result of fE_1.

4.3. Prediction of the shear modulus fG_{12}/fG_{13}

The prediction results of the tree depths of 6 and 7 are shown in Fig. 11. When the tree depth increased to 7, the error rate and RMSE/AV decreased. As the tree depth increased further, the reduction of the error rate and RSEM were not significant. Thus, the decision tree model with a tree depth of 7 was selected for the fG_{12}/fG_{13} prediction.

4.4. Prediction of the shear modulus fG_{23}

The prediction results of the tree depths of 6 and 7 are shown in Fig. 12. When the tree depth increased to 7, the error rate and RMSE/AV decreased. As the tree depth increased further, the reduction of the error rate and RSEM were not significant. Therefore, the decision tree model with a tree depth of 7 was selected for the fG_{23} prediction.

5. Conclusion

In this study, a new approach for predicting carbon fiber mechanical properties is proposed based on machine learning. The mechanical properties of the CFRP are determined by the mechanical properties of the fiber and matrix under a specified structure. Therefore, there is a correlation between CFRP and fiber/matrix; however, the relationship is complicated. This study establishes this relationship through a cross-scale finite element model, and then generates data samples by calling the non-GUI pattern through Software Isight. The regression tree model is used for feature selection, model training, and sample verifying. Using [0/90°] CFRP as an example, the properties of the carbon fiber were analyzed, and the conclusions are as follows.

1) Longitudinal elastic modulus fE_1. The elastic modulus of CFRP E_1 has a significant effect on fE_1, while the other feature effects are nearly negligible. The decision tree model with a tree depth of 3 is suitable for the fE_1 prediction.
2) Transverse elastic modulus fE_2/fE_3. The elastic modulus of CFRP E_3 and the elastic modulus of matrix mE have a significant effect on fE_2, while the other feature effects are individually smaller. The decision tree model with a tree depth of 7 is suitable for the fE_2/fE_3 prediction.
3) Shear modulus fG_{12}/fG_{13}. The shear modulus of CFRP G_{12} and the elastic modulus of matrix mE have a significant effect on fG_{12}, while the other feature effects are individually smaller. Therefore, the decision tree model with a tree depth of 7 is suitable for the fG_{12}/fG_{13} prediction.
4) Shear modulus fG_{23}. The shear modulus of CFRP G_{12} and G_{23} and the elastic modulus and Poisson's ratio of matrix mE and $m\nu$ have a significant effect on fG_{23}. The decision tree model with a tree depth of 7 is suitable for the fG_{23} prediction.

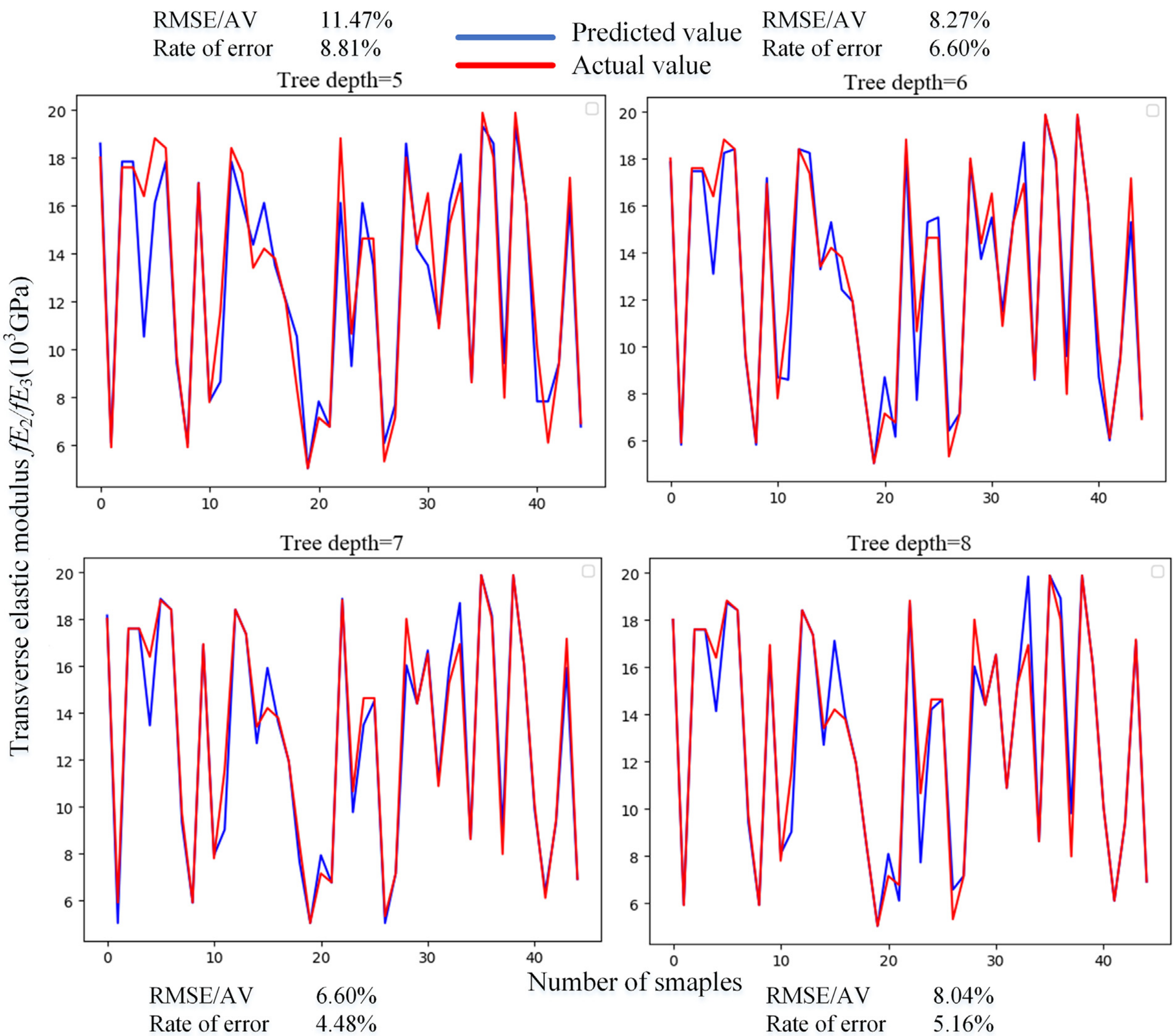

Fig. 10. Prediction result of fE_2/fE_3.

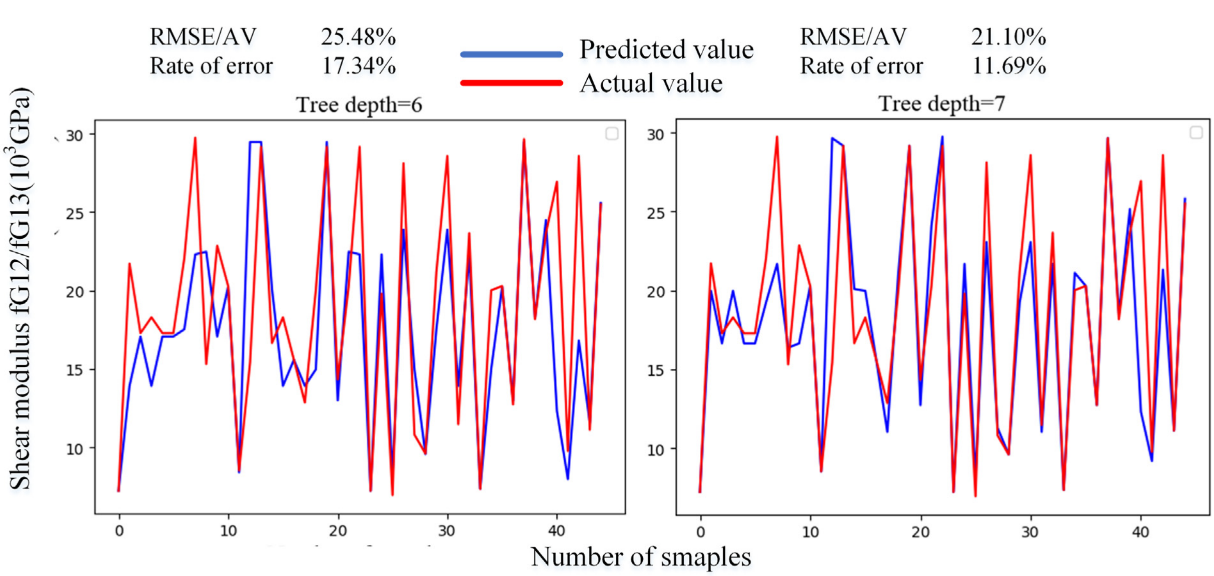

Fig. 11. Prediction result of fG_{12}/fG_{13}.

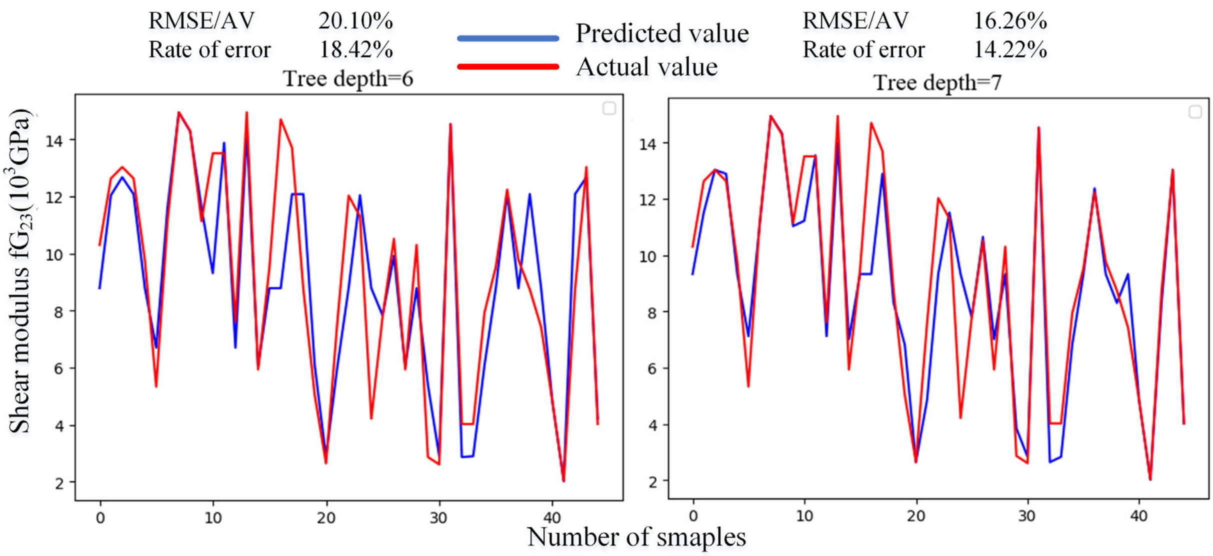

Fig. 12. Prediction result of fG_{23}.

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