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Machine Learning-Based Flexural Strength Prediction of Layered Ceramic Materials

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Abstract. The flexural strength of layered ceramic materials plays an important role in its application, and are affected by many structural parameters and process factors. At present, the experimental methods of layered ceramic materials are inefficient, and it is impossible to systematically analyze the effect of structural parameters and process factors on the bending strength of silicon nitride ceramics. In this paper, a machine learning model based on 3 classical algorithms is successfully established, and its bending strength is predicted with 5 indexes. According to the SHAP diagram, the material of layered ceramics has the greatest influence on the bending strength, followed by the sintering temperature, this article provides the basis and reference for the preparation of layered ceramic materials with high bending strength.

Keywords: Machine learning; layered ceramics; strength prediction.

1. Introduction

As a kind of excellent material, ceramics has many advantages, such as high hardness, good wear resistance, high temperature strength, good chemical stability, good dielectric corrosion resistance and excellent insulation performance. However, due to its low plasticity, poor strength, brittle fracture and other shortcomings, but also limited its scope of use. Biomimetic materials, inspired by the structure, function and properties of organisms, can effectively improve the plasticity of materials, and their applications in the field of ceramics have attracted increasing attention [1-4]. In 1990, Clegg et al. first proposed that the toughness of laminated ceramic composites could be greatly improved by using a pearl-like shell structure, by adding high temperature resistant soft materials into the brittle ceramic materials, the lamellar composite ceramics can improve the ceramic toughness and strength simultaneously [5].

Wei Chen used hot pressing to produce laminated Si3N4-Mo composites, and verified that the multilayer structure can improve the fracture toughness, and the higher Mo is conducive to hindering the crack diffusion and improving the fracture toughness of the material, but the singleness of the material and production method makes the experimental results unable to be generalized [6]. Rajendar Katla studied the effect of the composition of h-BN and B4C reinforcements on the properties of aluminum matrix composites (AMCs) and fabricated 10 AMCs with different reinforcements to study the effect of the reinforcements, but the control of their multi-component components was significantly more difficult to operate [7].

The previous research is often based on the limited structure characteristics, and the importance of the structure characteristics is not given a quantitative description, the ceramic layer material design guidance role is limited. Ceramic laminated materials include a variety of structural features (Substrate layer thickness, layer thickness ratio, layer number, different structural features, different preparation methods have different effects on the properties of the final materials. In order to solve the above problems, this article establishes a machine learning model based on three classical algorithms and predicts its bending strength with five indexes, large volume to make up for the material structure in the real experiment, a single, fixed generation of the defects.

2. Establishment and solution of the model

2.1. Data collection and feature selection

The data sets used in this article are all from various published papers, mainly core journal papers or degree papers, summarized 105 groups of experimental data. According to the previous research, 4 important characteristics, such as layer thickness ratio, relative layer number (sample height ratio layer number), substrate layer thickness and interface layer thickness, are selected:

$$ratio = \frac{Thickness\ of\ matrix\ layer}{Interface\ layer\ thickness} \tag{1}$$

$$\frac{h}{t} = \frac{Total\ height\ of\ material}{Layer\ number\ of\ interface\ and\ substrate} \tag{2}$$

$$h_1 = Thickness\ of\ matrix\ layer \tag{3}$$

$$h_2 = Interface\ layer\ thickness \tag{4}$$

Considering that the above characteristics can not fully express the material information hidden behind the group elements, on the other hand, it is difficult to determine the composition and content of layered ceramic materials based on atomic scale characteristics, so the elements and content as well as molding technology, molding temperature, molding pressure, molding time into the machine learning feature space. In addition, principal component analysis (PCA) is used to reduce the dimension of components in order to avoid over-fitting caused by too many features. Finally, the feature space consists of nine typical features, it includes element and content, material layer thickness ratio, relative layer number (sample height ratio layer number), substrate layer thickness, interface layer thickness, molding technology, molding temperature, molding pressure, molding time.

2.2. Feature works

The goal of feature engineering is to transform the original data into a form more suitable for algorithm learning. The input variables in the data set constructed in this paper include continuous variables and unordered classification variables. For continuous variables, tree-structured models and naive Bayesian cognitive science do not require normalization and normalization of data sets compared with other ML algorithms. Therefore, just focus on unordered categorical variables. Considering that unordered classification variables can not be directly applied to model construction, label coding method is used to map the high cardinality classification variables to numerical variables. It should be noted, however, that elements and content characteristics can not be encoded directly, which would otherwise lead to confusion in element digitization, as the number of group elements in each case in this study was different and the order of elements was not differentiated. In order to avoid this situation, article refer to Jicheng Liu coding method [8]. In shown in Figure 1, merge the 7 column group elements into 1 column and replace the null value with 0. Based on this, the elements are digitized and the original data is replaced with tag encoding. Finally, to prevent the“Dimension curse”, article use PCA to merge multiple columns of elements and content into one column and name this feature element and content (E & C).

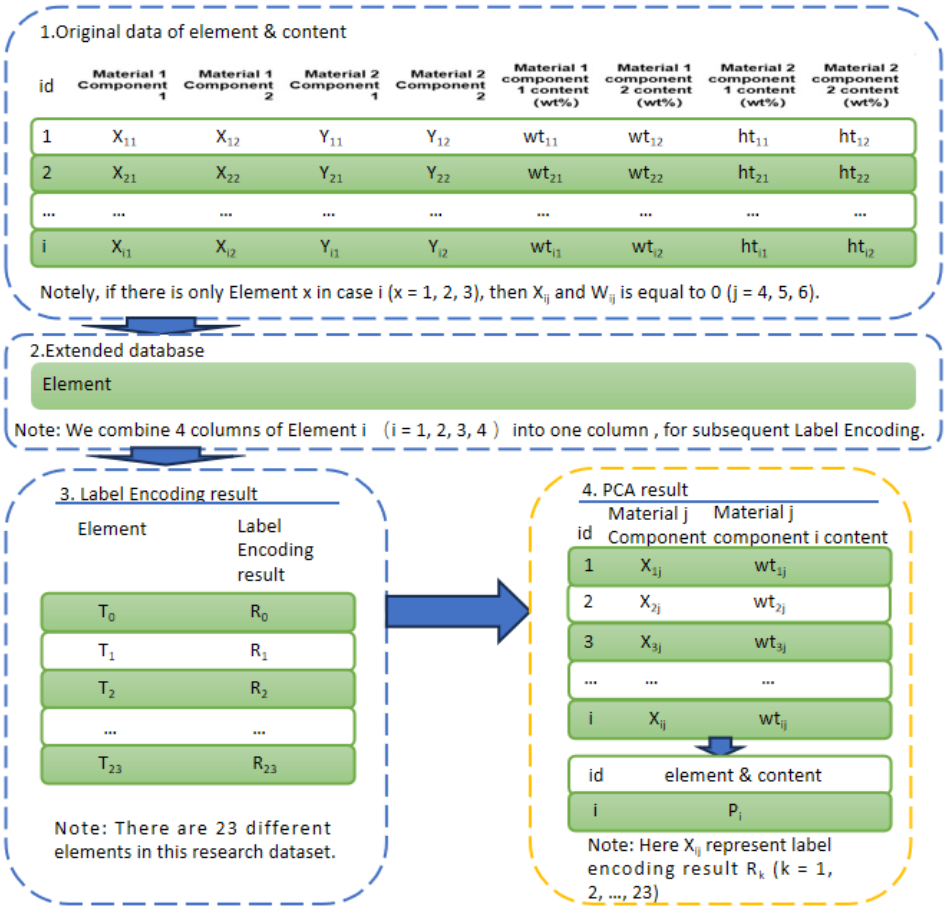

Figure 1. Process Flow diagram of coding group elements and contents

In addition, the classical over-sampling method-ADASYN data balance technique is used to solve the problem of unbalanced distribution of the original data set, in which the low-intensity, medium-intensity, there were 41,54 and 10 samples of high strength layered ceramic materials, respectively. The formula of the new composition algorithm (s_i) is as follows:

$$s_i = x_i + (x_{zi} - x_i) * \lambda \tag{5}$$

Where x_i is an example of a few classes of data, x_{zi} is the K nearest neighbor classification algorithm (KNN) for data and is a random number between 0 and 1. The advantage of most classes determines how many virtual samples are generated from each minority class sample using the KNN principle. Then, the balanced data set was divided into training set and test set in a 7:3 ratio.

2.3. Algorithm selection

Decision Tree and Naive Bayes are two common algorithms for classification problems, the former is represented by XGBoost and RF. The XGBOOST algorithm uses the idea of combining the integration algorithm with the decision tree, while the RF algorithm is based on the idea of combining the integration algorithm with the decision tree. Therefore, this research chooses these three representative classification algorithms (XGBoost, RF and NB) to carry on the modeling. Among them, XGBoost use simple, fast and efficient, RF is good at dealing with data imbalance classification problems, NB has a solid mathematical foundation and stable classification efficiency.

2.4. Assessment indicators

In this paper, the overall classification accuracy (ACC), recall rate, precision, F1 score, area under work characteristic curve (AUC) were used to evaluate the model. The formula is as follows:

$$ACC = \frac{TP+TN}{TP+TN+FP+FN} \tag{6}$$

$$Recall = \frac{TP}{TP+FN} \tag{7}$$

$$Precision = \frac{TP}{TP+FP} \tag{8}$$

$$F_1 = \frac{2TP}{2TP+FN+FP} = \frac{2 \cdot Precision \cdot Recall}{recision+Recall} \tag{9}$$

Among them TP, TN, FP and FN are confusion matrix parameters. In general, recall is negatively correlated with accuracy, whereas the F1 score takes both accuracy and recall into account. The value of AUC can intuitively evaluate the discriminant ability of the classifier, ranging from 0.5 to 1. An AUC of 1.0 indicates full ability to discriminate between positive and negative conditions, while an AUC of 0.5 indicates no ability to discriminate.

3. Results

3.1. Data set interpretation and imbalance correction

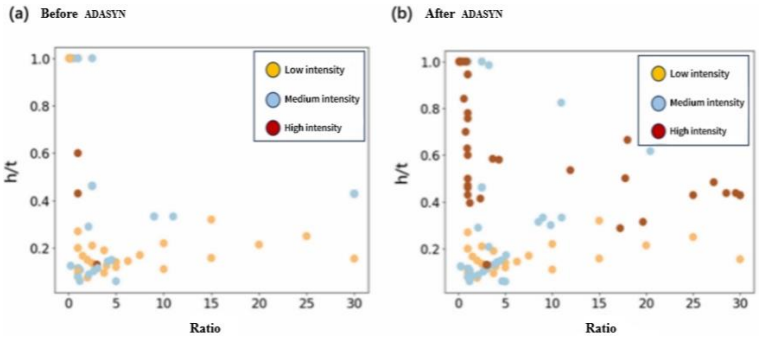

Figure 2. Data distribution of layer thickness ratio/relative layer number

After ADASYN oversampling, a new balanced data set (high intensity: 53, medium intensity: 54, low intensity: 60) was constructed. Figure 2 shows the difference in the distribution of the ADASYN data set between the thickness ratio/height ratio of the final material 1 and material 2 and the total number of layers of the sample height ratio, a large number of low-strength and high-strength data are generated adaptively near medium-strength data points.

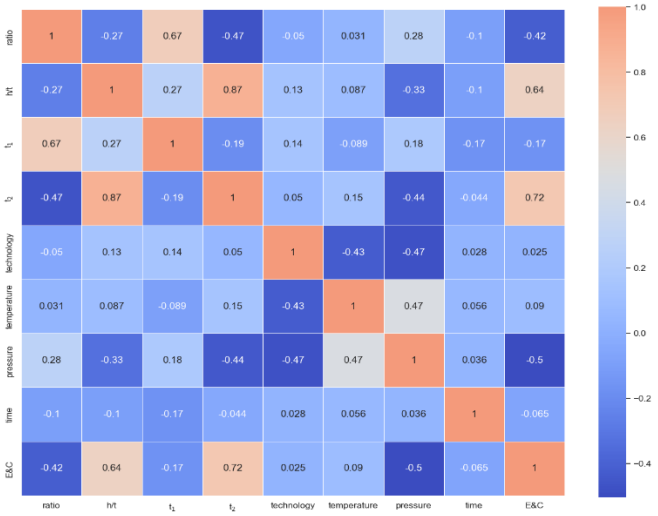

Figure 3. Pirsson product moment correlation heat map of input features

Figure 3 is Pearson product moment correlation coefficient (PCC) graph, the analysis quantifies the correlation between input features. The analysis shows that the strength of layered structure depends on many input characteristics. In other words, a single feature cannot be used to determine the strength of a layered material. Furthermore, as shown on the right in Figure 3, the PCC absolute value between most features was below 0.7, but the PCC absolute value was above 0.7 in the thickness-to-height ratio of the feature material II to the number of layers; However, according to the relevant literature, there is no obvious correlation between the two, so, after comprehensive consideration, the two characteristics are retained, other PCC absolute values all indicated no strong correlation between the nine features of the input [9].Therefore, in the end, article propose to use all nine features to participate in the machine learning process.

3.2. Classification performance comparison and model analysis

Three classical machine learning algorithms (XGBoost, RF and NB) were selected to construct the prediction model. Before the training model, the balanced data set was randomly divided into the training set and the test set in a 7:3 ratio. Then, the parameters of the model are optimized by repeated triple cross-validation and super-parameter tuning. Table 1 and Table 2 list the XGBOOST and RF tuning parameter space and optimal parameter selection, respectively. It should be noted that NB algorithm is based on Bayesian formula and does not need hyperparameter tuning.

Table 1. Detailed parameter configuration for XGBoost superparameter tuning

Parameters	Initialization value	Search space	Optimal value
n_estimators	400	[500, 600, 700]	700
min_child_weight	1	[1, 2, 3]	1
max_depth	5	[3, 4, 5]	4
Subsample	0.6	[0.5, 0.6, 0.7]	0.7
colsample_bytree	0.7	[0.5, 0.6, 0.7]	0.5
learning_rate	0.1	[0.01, 0.02, 0.05]	0.02

Table 2. Detailed parameter configuration for RF superparameter tuning

Parameters	Initialization value	Search space	Optimal value
n_estimators	10	[500, 600, 700]	500
max_leaf_nodes	None	[5, 10, 15]	15
max_depth	None	[3, 4, 5, 6, 7]	7
min_samples_leaf	1	[1, 3, 5]	1
min_samples_split	2	[1, 3, 5]	3

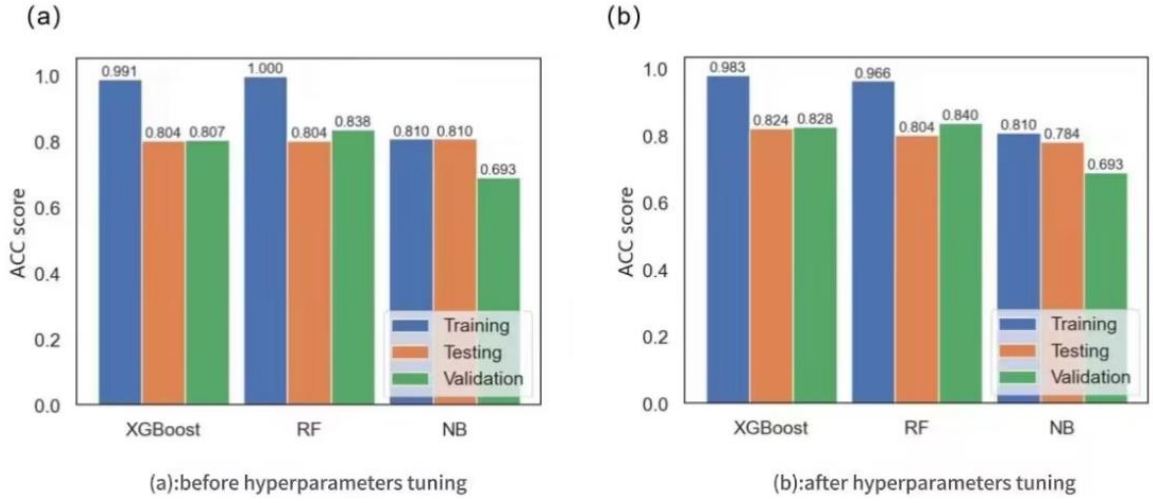

Figure 4. ACC comparison of training set, test set and verification set

Figure 4 shows the accuracy (ACC) of the untuned and tuned models implemented throughout the training, testing, and validation process. It is clear that the accuracy of the RF model is better in the validation set than in the other two models. Notably, the tuning of the XGBOOST algorithm increased the ACC of the test set and the validation set by approximately 2% and 2.1%, respectively, to 82.4% and 82.8%, essentially the same as the RF model on the test set; However, it is still inferior to the RF model in the verification set. In contrast, the ACC of the NB model was lower than that of the optimized XGBoost and RF models across all data sets, and in particular the accuracy of the validation set was less than 70%. In addition, as shown in Table 3, the NB model and the RF model also had lower F1 scores, accuracy, recall and AUC than the XGBoost and RF models, and the accuracy of the models was not guaranteed, so the XGBOOST model was selected for the final analysis.

Table 3. Performance of models built using different classifiers

Algorithm	F1 score	AUC	Precision	Recall
XGBoost	0.824	0.959	0.832	0.824
RF	0.804	0.951	0.805	0.805
NB	0.784	0.891	0.792	0.786

3.3. Feature analysis

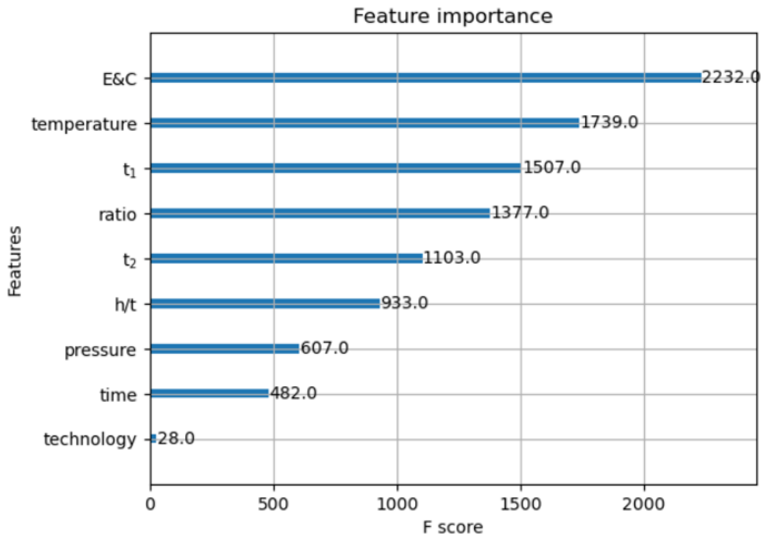

Figure 5. XGBoost feature importance analysis diagram

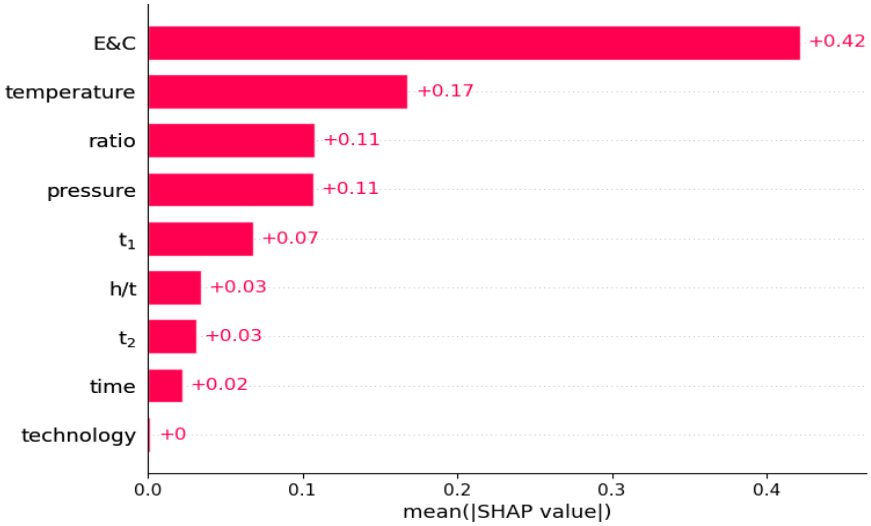

Figure 6. SHAP bar chart

Figure 5 shows the results of the important analysis that comes with the XGBOOST model, while Figure 6 represents the corresponding SHAP addition interpretation (SHAP) bar graph to explain the XGBoost-built black box model [10]. It is found that the sintering pressure affects the properties of the ceramic lamellar materials mainly by affecting the density and the interface strength, but the effect is small, therefore, article believe that the effect of sintering pressure on the properties of layered materials should be based on the characteristic importance analysis of the XGBOOST model. Then article compare the two figures. In the two figures, the material of lamellar material has the most influence on the bending strength, and the second is the preparation temperature. The sintering temperature can change the density and grain size of the material, and then affect the mechanical properties of the material, grain size increases with the increase of temperature. The mechanical properties of Al_2O_3/W laminated composites are related not only to the thickness of ceramic and metal layers, but also to the thickness ratio of ceramic/metal layers. The flexural strength of Al_2O_3/W laminated composites increased with the increase of the lamellar thickness ratio, while the fracture toughness decreased. By studying the effect of layer thickness ratio and layer number on Al_2O_3/Ni laminated composites, it is found that fracture toughness and fracture work decrease with the increase of layer thickness ratio, The maximum values reached 12.56 $MPa \cdot m^{0.5}$ and 12450 J/M^2 [11].

As for the effect of sintering time, it is well known that sintering time has a certain relationship with the density of ceramic materials. The density of ceramic materials is closely related to their properties, so the sintering time has some effect on the ceramic layer materials. At the same time, article notice that the effect of the preparation method on the ceramic lamellar materials is small, because the preparation method of ceramic lamellar materials is mainly hot-pressed sintering, so the difference of input data is not significant.

4. Conclusion

Based on the study of the strength of layered ceramics, this paper obtains the importance degree of the related characteristics that determine the strength of layered ceramics through the correlation comparison of various characteristics, then the temperature of sintering ceramics, the related parameters of substrate layer and interface layer, such as thickness and proportion, and finally the least influence is the sintering time and the preparation method, by adjusting the related parameters of its characteristics, it can change the strength of layered ceramic more effectively and provide guidance for the preparation of ceramic materials.

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