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Tensile property prediction by feature engineering guided machine learning in reduced activation ferritic/martensitic steels

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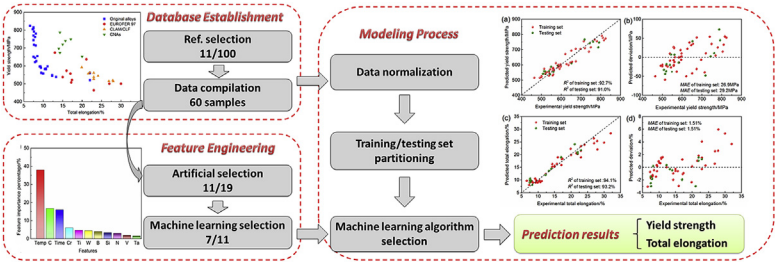
HIGHLIGHTS

- A tensile property database of RAFM steels was established.
- High correlated features were selected to train the random forests regressors.
- Both yield strength and total elongation of RAFM steels were predicted.
- The process window of RAFM steels for reasonable tensile property was calculated.

GRAPHICAL ABSTRACT



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ABSTRACT

The accurate prediction of tensile properties has great importance for the service life assessment and alloy design of RAFM steels. In order to overcome the limitation of traditional physical metallurgical models, machine learning algorithm was used to establish universal models for the prediction of RAFM steels' yield strength and total elongation. A database with a wide range of compositions and treatment processes of RAFM steels was first established. Then, feature engineering methods were used to select the highly correlated features. With the reasonable selection of machine learning algorithm and test/training set partitioning strategy, random forests regressors were trained by the selected features. The prediction results proved that, compared with traditional physical metallurgical models, the feature engineering guided random forests regressors had advantages of accuracy and universality for the prediction of RAFM steels' yield strength and total elongation. And the calculated process window for the balance of strength and plasticity could provide guidance for the further design and development of RAFM steels.

1. Introduction

Reduced activation ferritic/martensitic (RAFM) steels for fusion reactor structural applications have been focused and developed for several decades because of their inherently excellent properties, such as strength, thermal conductivity, and irradiation resistance, compared with those of austenitic stainless steels [1–3]. As a structural metal material, tensile properties are also the basic factors, which have high priority during the design and service evaluation process for RAFM steels. Therefore, in order to reduce the time and cost of preparation and testing, computation models have been widely established and developed for the tensile property prediction of RAFM steels for long periods.

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Before the development of RAFM steels, tensile property prediction was already a long-standing topic in the field of metal materials. Based on classical mean-field dislocation theory, traditional physical metallurgy models were established and widely used. They included Peierls-Nabarro (P–N) model for P–N stress [4], Hall-Petch model for grain refinement strengthening [5,6], Kocks-Mecking model for dislocation interaction strengthening [7,8], Orowan dislocation looping model [9] and Friedel's shear cutting model [10] for precipitation strengthening, etc. Finally, all the traditional strengthening models could be combined by superposition law and obtain the yield strength of the steels with multi-method strengthening. Both G.B. Olson in Northwestern University [11] and E.I. Galindo-Nava in University of Cambridge [12] used this kind of superposition models to predict the yield strength of ultra-high strength steels and guide the further optimization and design. In view of Olson and Nava's results [11,12], the superposition models were further modified as a multi-scale model by considering the effect of both temperature and irradiation in Wang's work [13]. This multi-scale model was used to simulate both yield strength and irradiation hardening phenomenon in RAFM steels. Although physical metallurgy models based on mean-field dislocation theory obtained series of remarkable achievements for the yield strength simulation, plastic stage is still a serious problem because plasticity is a complex process, which is not only depended on dislocation multiplication [14]. So, in order to deal with plasticity, several researches used finite element method (FEM) to simulate the constitutive relationship of mechanical properties or microstructure-mechanical properties during plastic deformation [15,16]. The constitutive behavior of RAFM steels under irradiation conditions were simulated by FEM in J. Aktaa's work [15] and more tensile property information was obtained instead of only yield strength.

As mentioned above, after long-period development, traditional methods for tensile property simulation based on dislocation theory or constitutive relationship obtained great results and helped to reveal the strengthening mechanism of RAFM steels. However, with the deepening of research, the strengthening mechanism of RAFM steels was founded to be more and more complex. It meant that the constitutive equations in these models became more complicated and more parameters with fitting values should be used. So, in order to improve the accuracy of the models by the precise description of strengthening mechanism, the complexity of the traditional models seriously restricted their universality. However, the prediction of properties or the design of new alloys needed models with wide applicability, which could maintain the stability and accuracy in large range of composition and treatment condition. It meant that, nowadays, traditional models based on dislocation theory or constitutive relationship were more suitable for simulation or mechanism explanation, instead of prediction or alloy design [17].

For the situation mentioned above, several researches tried to develop the models suitable for tensile property prediction and alloy design, which meant the models didn't focus on complex physical mechanism, but paid close attention to the universality [18,19]. A. Tavassoli [18] arranged large amount of data for reduced activation martensitic steel, and established several fitting equation to predict the mechanical properties in a large range of temperature and irradiation condition. However, succinct fitting equations couldn't accurately express the complex relationship between properties and critical factors. So, as a well-known effective method for expressing universal relationship in large amount of complex data, machine learning algorithm began to be used [20]. In R. Kemp's work [19], an artificial neural network was used to express the irradiation hardening of low-activation ferritic/martensitic steels. A database of the tensile properties of various kinds of RAFM steels was compiled for the training of artificial neural network and the composition and treatment condition information was selected as 37 features for training the model. The model showed relatively better universality than the traditional models based on physical mechanism. However, its training approximation and generalization ability was still not as good as expected. In fact, traditional machine learning algorithms were already used for tensile strength prediction in several different kinds of steels (as pipeline steels, TRIP steels, etc.) and obtained promising results [21–26]. However, the situation of RAFM steels was quite different with them. The training approximation and generalization ability of machine learning models was significantly depended on the amount and quality of the data used for training. However, the sensitivity of the application limited the amount of data for RAFM steels. Also, the usage of microelements (as B, N, Ta, etc.) which were difficult to be tested limited the quality of data for RAFM steels. So, it was extremely difficult to predict tensile properties of RAFM steels well only by traditional machine learning algorithm without artificial guidance. In order to establish an effective machine learning model for RAFM steels' tensile property prediction, data should be further analysis and artificial guidance or constraint should be added to modify the traditional machine learning algorithm. For example, using feature engineering treatment to tell the models how to select the useful features and ignore the useless ones [27].

In this work, feature engineering idea was used to guide the modification of machine learning algorithm. And the modified machine learning models were used to predict the tensile properties of RAFM steels. The analysis of the results could provide guidance for the application of machine learning algorithm in property prediction and alloy design of RAFM steels.

2. Modeling process

The framework of the feature engineering guided machine learning system was schematically illustrated in Fig. 1. As the premise of the calculation by machine learning algorithm, an original database was firstly established. Then, in order to improve the quality of the database, feature engineering was used to select the highly correlated features and a modified database was obtained. For the modified database, normalization was used as data preprocessing method to eliminate dimensional differences

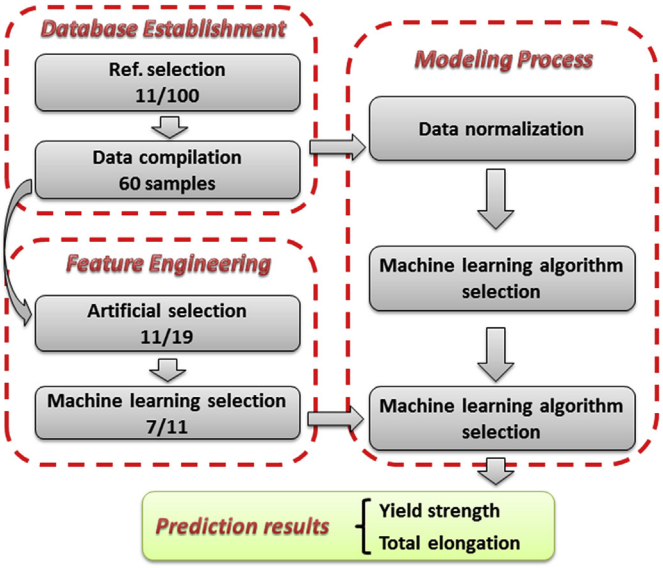

Fig. 1. Framework of the feature engineering guided machine learning system.

between inputs. Finally, after the selection of machine learning algorithm and test/training set partitioning strategy, the modified database were divided into a training dataset (80%) and a test dataset (20%) and feature engineering guided random forests regressors (FE-RFRs) were trained for the prediction of both yield strength and total elongation of RAFM steels.

3. Calculation results

3.1. Database and feature engineering

For the original database, ~100 references were first collected. After careful consideration of the comparability, 11 of them were used for the establishment of original database [28–38]. The original database included 60 samples of RAFM steels with all the information of composition, treatment process, and conventional mechanical properties. As shown in Fig. 2, Both traditional RAFM steels in different countries (as traditional/modified Eurofer97 in Europe, traditional/modified CLAM in China, etc.) and new developed prototype alloy by different research institute (as CNAs by Oak Ridge National Laboratory, M-RAFM in Tsinghua University, etc) were included in the original database with relatively uniform distribution of the properties.

Based on the original database, feature engineering was used to further improve the quality and analyzability of the database. For any machine learning algorithm which targeted to the prediction of material property, it should depend on features (descriptors). As important inputs of machine learning models, the features strongly related to the prediction results. For a complex problem, the amount of the features could be extremely large. However, with the limitation of data, the number of features used in machine learning models should be reasonably controlled. The best strategy was to choose features that perfectly represented the materials' property and the number of features should be far less than the number of samples in database to avoid the curse of dimensionality [27]. In this work, the feature engineering process included two stages: artificial selection and machine learning selection. For the original database, 19 initial features were included. Firstly, by considering the data quality, 8 features were ignored artificially. The 8 ignored features included the content of Mo, Ni, Nb, Mn, V (The data range was too narrow), the content of P, S (Doubts about data quality because of the testing accuracy) and the austenitizing temperature/time (data amount was too small). Then the 11 remaining features were used for the further selection. After the artificial feature selection, the inputs of the modified database were shown in Table .1.

For the machine learning selection progress, the random forests (RF) algorithm was used to evaluate the importance of the 11 remaining features quantitatively and "last-place elimination" rules were further used to efficiently exclude the features which had less effect on the property prediction.

The calculated importance and correlation of the selected features for the yield strength of RAFM steels was shown in Fig. 3(a) and (b). The results showed that the tempering temperature took the most important role on the yield strength prediction, followed by the content of C, tempering time, the content of Cr, Ti, W and B (Fig. 3(a)). It was worth noting that the importance of tempering temperature, time and C content was significantly higher than other features. These results were basically consistent with the principles of traditional physical metallurgy and previous understand of RAFM steels. RAFM steel was a kind of aging steel with precipitation strengthening as the main strengthening mechanism and the main contributor of the strength was the MX carbonitride, which was mainly formed during tempering [13]. So, it was reasonable that tempering process and C content was critical for the yield strength of RAFM steels. Pearson correlation coefficient matrices were calculated to express the positive and negative correlations between pairs of features (Fig. 3(b)). The low linear correlations for most of features indicated that, by using the top 7 important features, redundant and negligible features were successfully removed, which would probably help to improve the performance of the machine learning algorithm.

Similar with the feature analysis for yield strength, the calculated importance and correlation of the selected features for the total elongation of RAFM steels was also shown in Fig. 3(c) and (d). The results showed that the tempering time took the most important role on the total elongation prediction, followed by the content of Cr, Ta, N, W, Si and C (Fig. 3(c)). It was reasonable that the plasticity could be significantly affected by the tempering time and Cr. Based on the previous experimental results of RAFM steels, plasticity of RAFM steels had strong relationship with the coarsening of $M_{23}C_6$ at the grain boundary. Because Cr was the main alloy element of $M_{23}C_6$ and $M_{23}C_6$ usually had large coarsening rate during the tempering, tempering time and Cr could affect the total elongation of RAFM by $M_{23}C_6$ [13]. Also, similar with the feature analysis for yield strength, redundant and negligible features were successfully removed by using the top 7 important features for total elongation (Fig. 3(d)).

3.2. Prediction results

After the analysis of feature engineering, 7 most important

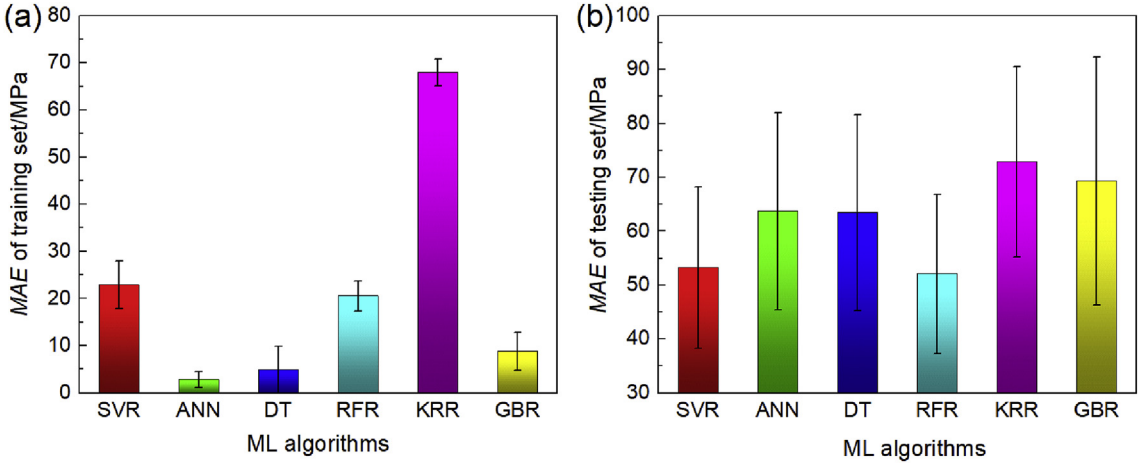

Fig. 2. Visualization of the original database in this work.

Table 1
Inputs and outputs information for the modified database.

	Inputs and output	Maximum	minimum	mean	Standard deviation
Inputs	C (wt.%)	0.13	0.03	0.10	0.02
	Cr (wt.%)	9.30	4.61	7.71	1.74
	W (wt.%)	3.01	0.00	1.84	0.70
	Si (wt.%)	0.77	0.00	0.16	0.11
	V (wt.%)	0.30	0.05	0.23	0.04
	Ta (wt.%)	0.55	0.00	0.08	0.08
	Ti (wt.%)	0.15	0.00	0.01	0.04
	N (wt.%)	0.43	0.00	0.02	0.06
	B (wt.%)	0.01	0.00	0.001	0.003
	Temp (°C)	780.00	650.00	737.87	27.88
	Time (min)	120.00	30.00	74.00	29.23
Outputs	YS (MPa)	824.00	464.00	621.44	99.57
	TE (%)	32.00	6.60	15.01	6.96

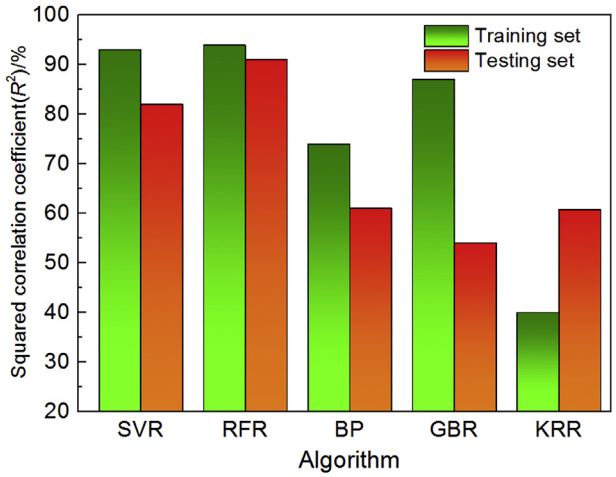

Fig. 3. Importance and correlation of the features: (a) ranking of the features for yield strength prediction; (b) Pearson correlation coefficient matrix among the features for yield strength prediction; (c) ranking of the features for total elongation prediction; (d) Pearson correlation coefficient matrix among the features for total elongation prediction.

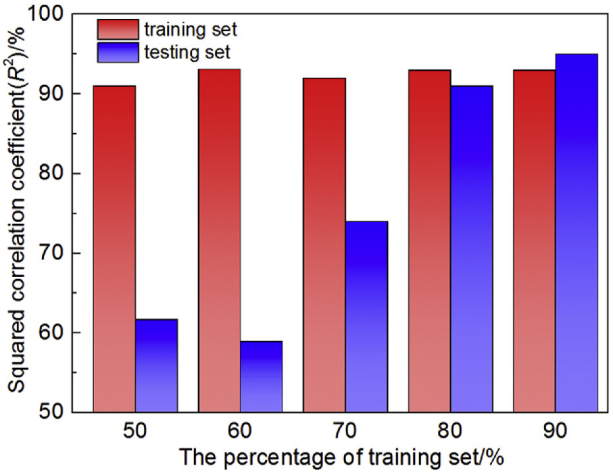

Fig. 4. Prediction results by FE-RFRs (a) prediction results of yield strength; (b) MAE of the yield strength prediction; (c) prediction results of total elongation; (d) MAE of the total elongation prediction.

features are sorted out from the 11 remaining features and constitute as an optimal feature set. Then, random forests regressors (RFRs) were trained by the optimal feature set for the prediction of both yield strength and total elongation of RAFM steels. The feature engineering guided RFRs (FE-RFRs) included 100 decision trees and the max depth of the decision trees was set as 5. The prediction results of yield strength were shown in Fig. 4(a) and (b). Squared correlation coefficient (R^2) between experimental value and predicted value was used to evaluate the predicted accuracy. Both training and testing set showed high value of R^2 (>90%), which meant that the model had no overfitting or underfitting problem and it could probably make relatively accurate prediction of the yield strength (Fig. 4(a)). Fig. 4(b) showed that, for all the 60 samples in the database, the mean absolute deviation (MAE) of the yield strength prediction results was less than 30 MPa. It indicated that feature engineering guided machine learning models could obtain better accuracy and universality than previous multi-scale models based on physical metallurgy (MAE = 50 MPa for 8 samples) [13].

Also, the prediction results of total elongation of RAFM steels by FE-RFRs were shown in Fig. 4 (c) and (d). Similar with FE-RFRs for yield strength, FE-RFRs for total elongation also showed high value of R^2 (>90%) for both training and testing set (Fig. 4(c)). Also, the MAE of the total elongation prediction results was only about 1.5%, which meant that the FE-RFRs for total elongation had even better performance than the FE-RFRs for yield strength (Fig. 4(d)). Restricted by the complex and controversial plastic deformation mechanism, the prediction of elongation was a long-standing problem in the field of physical metallurgy modeling. So, the FE-RFRs used in this work could not only be used for the RAFM steels' property prediction, but also provide new ideas for plasticity simulation in the field of other metal materials.

In summary, with the guidance of feature engineering, the trained FE-RFRs showed gratifying accuracy and universality for the prediction of RAFM steels' tensile properties. They could be used to predict the yield strength and total elongation of RAFM steels in a wide range of compositions and treatment processes. In the range of 0.03–0.13 wt %C, 4.61–9.30 wt % Cr, 0–3.01 wt % W, 0–0.77 wt % Si, 0.05–0.3 wt % V, 0–0.55 wt % Ta, 0–0.15 wt % Ti, tempering temperature 650–780 °C, tempering time 30–120 min, the prediction error of FE-RFRs could probably be <5% for both yield strength and total elongation. This modeling framework could be considered as a new strategy for the quantitative guidance of the alloy design of RAFM steels.

4. Discussion

4.1. Selection of machine learning algorithm

As one of the main topic in machine learning, supervised

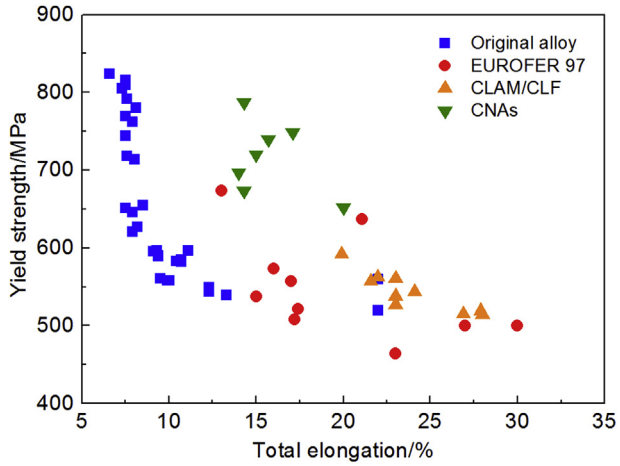

Fig. 5. Squared correlation coefficient for different machine learning algorithms.

learning was studied in decades and various kinds of regressors were developed, as back propagation artificial neural network (BP-ANN) [39], support vector regressor (SVR) [40], random forests regressor (RFR) [41], Gradient boosting regressor (GBR) [42], Kernel ridge regressor (KRR) [43], etc.. Every regressor had its advantages and characteristic of dealing with different kinds of database. So, the selection of regressor types should be considered before the establishment of the whole structure of machine learning prediction system. Before RFRs were used as the main machine learning algorithm for the tensile property prediction of RAFM steels, most traditional regressors were tested and the results of R^2 for both training and testing set were shown in Fig. 5. It was clear that, as an efficient algorithm which was usually good at dealing with high-dimensional data, SVR showed better performance than most other traditional regressors. However, for the database in this work, RFR showed even better performance than SVR. For the database used in this work, SVR still showed slight over-fitting, as the R^2 for training set was about 10% larger than that for testing set by SVR. Similar with SVR, RFR was also good at dealing with high-dimensional data. In addition, by combining large amount of decision trees, RFR had better ability to overcome the over-fit problem than SVR. So, RFR was selected as the optimal machine learning algorithm in this work.

4.2. Selection of test/training set partitioning strategy

In order to avoiding underfitting or overfitting problems, the selection of test/training set partitioning strategy was always the key point for the training of machine learning models. With different partitioning ratio, the effect of test/training set partitioning strategy on the performance of RFRs was analyzed as Fig. 6. For the database used in this work, when the percentages of training set were less than 80%, the R^2 for training set was much larger than testing set, which represented a serious over-fitting. When the percentages of training set were equal to 80%, R^2 for both training and testing set was relatively balanced. And when the percentages of training set were more than 80%, the R^2 for testing set became slightly higher than training set, which indicated the slight trend of under fitting. So, as mentioned in section 2, 80% data for training set was finally used as the optimal test/training set partitioning strategy in this work.

4.3. Comprehensive analysis of the prediction results

As mentioned in section 3.1, the top two important features for

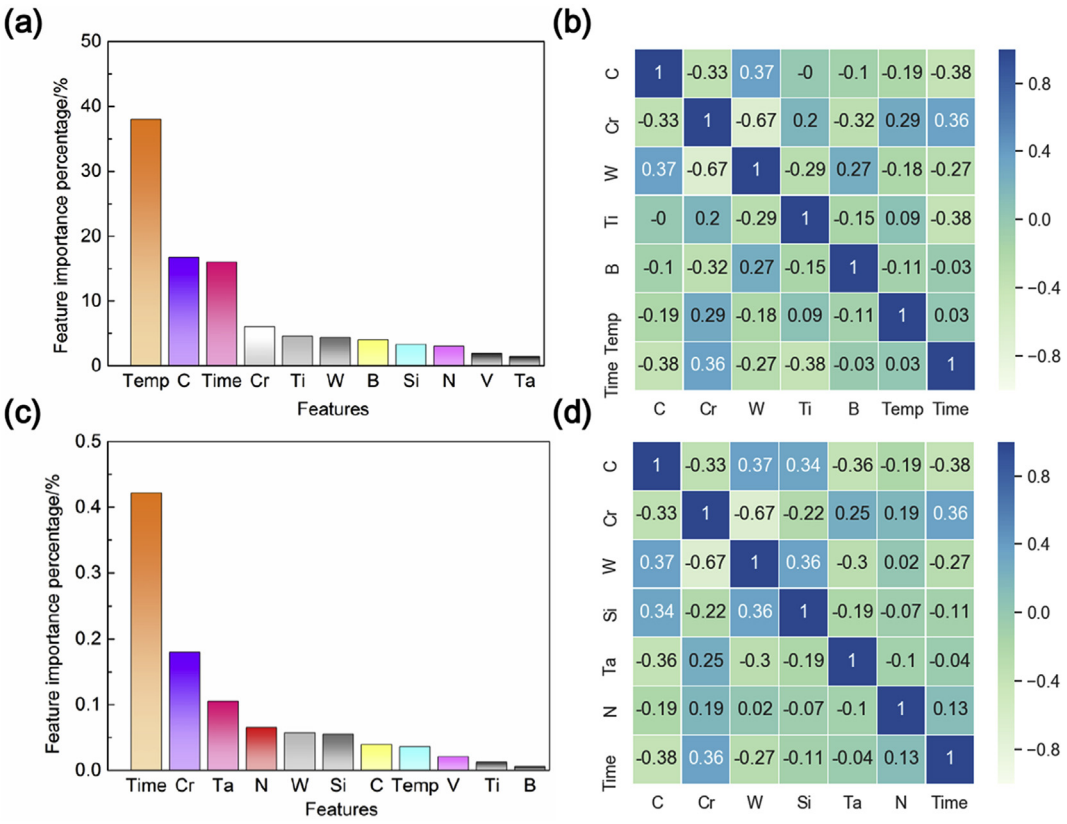

Fig. 6. Squared correlation coefficient for different test/training set partitioning strategy.

yield strength and total elongation was respectively tempering temperature, C content, tempering time, and Cr content. In order to make further understanding of the prediction results, the effect of these four features on tensile properties were comprehensive analyzed as Fig. 7. As shown in Fig. 7(a), relatively higher yield strength could be obtained when the C content was about 0.06–0.08 wt% and the tempering temperature was in the range of 670–760 °C. In that situation, if the total elongation was further considered, the tempering temperature should be limited in the range of 750–760 °C (Fig. 7(b)). Relatively higher tempering temperature (>760 °C) would lead to the insufficient yield strength (<460 MPa) and relatively lower tempering temperature (<750 °C) would lead to the insufficient plasticity (total elongation<15%). So, the prediction results indicated that, in order to obtain good balance between strength and plasticity, the tempering temperature should be fixed at about 750–760 °C. This was also consistent with the standard treatment process of most RAFM steels, like F82H, Eurofer97, CLAM, etc. [32–36]. However, for tempering time and Cr content, relatively larger ranges were available. As shown in Fig. 7 (c) and (d), for a good balance of strength and elongation, the range of tempering time could be 30–120 min and the Cr content could be 8–9 wt %, which was also reasonable based on the traditional physical metallurgy theory and previous experimental results of RAFM steels [13]. So it provided an appropriate design space for other properties, as the irradiation resistance, creep, etc.. For the further development and design of the new generation of RAFM steels, this process window could be used as the reference for the design of the composition and treatment process.

In summary, although several prospective results were shown in this work for the RAFM steels' tensile property prediction, the feature engineering guided machine learning prediction system used in this work was only a preliminary attempt for how to use feature engineering idea to modify the performance of machine learning algorithm in the field of RAFM steels. The main idea of feature engineering was to select and obtain the most useful features, not only remove the useless one as shown in this work, but also introduce the critical features which shouldn't be ignored. As well-known, the properties of steels critically depended on microstructures. However, in most previous researches by traditional machine learning algorithms, only composition and treatment process were used as features. It was reasonable that, if more microstructure information could be added as the features, they could probably give more useful guidance for improving the performance of machine learning algorithms. As shown in Fig. 8, for the further researches, microstructure information (as phase fraction, driving force, growth rate, etc.) could be calculated by various thermodynamic simulation methods and used as the features for the machine learning prediction of various properties in different steels. So, based on the results in this work, more meaningful researches could be made in the field of feature engineering guided machine learning. They could be not only for tensile property prediction, and also not only for RAFM steels.

5. Conclusion

In this work, a database covered a wide range of compositions and treatment processes of RAFM steels was established. Based on the database, feature engineering guided random forests regressors were trained and used to predict the tensile properties of RAFM steels, including yield strength and total elongation. The main points of this paper were as follows:

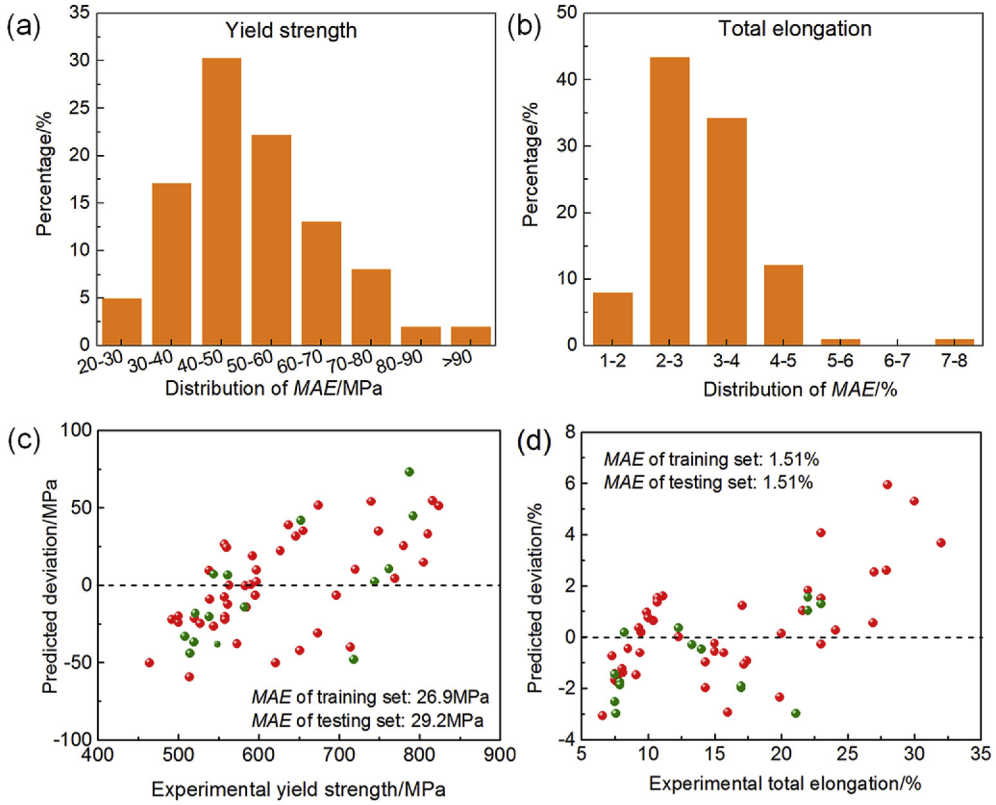

Fig. 7. Comprehensive analysis of the prediction results: (a) contour map of yield strength with the factors of tempering temperature and C content; (b) contour map of total elongation with the factors of tempering temperature and C content; (c) contour map of yield strength with the factors of tempering time and Cr content; (b) contour map of total elongation with the factors of tempering time and Cr content.

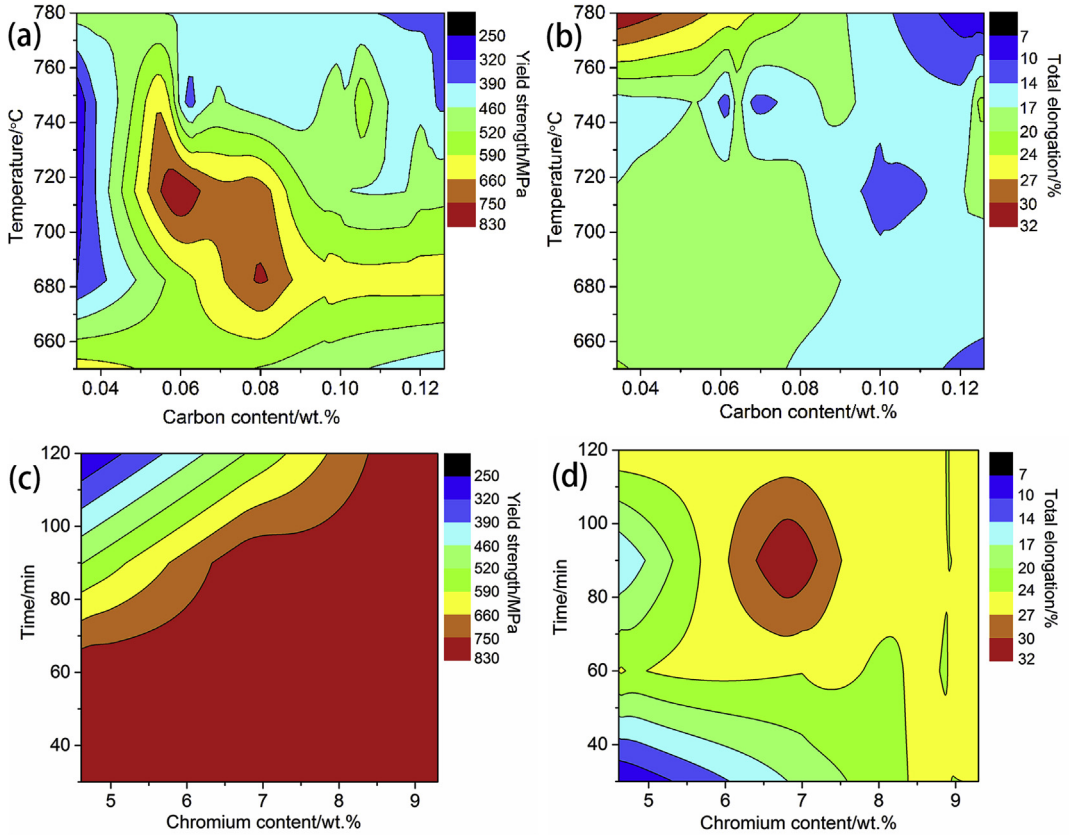

Fig. 8. The prospect of feature engineering guided machine learning for steels.

(1) A machine learning modeling framework, which included the database, feature engineering, model selection and training, was established and proved to be suitable for the universal prediction of tensile properties in the field of RAFM steels. It also provided a useful mode for the prediction of other properties in the field of RAFM steels.
(2) With the help of feature engineering, the high correlated features could be found, as tempering temperature and C content for yield strength and tempering time and Cr content for elongation. The sorting of features by the importance could effectively guide the training process of machine learning models and improve the performance of the models for the prediction of RAFM steel's tensile properties.
(3) By the reasonable selection of machine learning algorithm and test/training set partitioning strategy, feature engineering guided random forests regressors were trained for the prediction of RAFM steels' tensile properties. The trained models showed significantly higher accuracy and universality than traditional physical metallurgical model.
(4) Based on the prediction results, a process window of RAFM steels for the balance of strength and plasticity was established (tempering temperature 750–760 °C, tempering time 30–120mins, Cr content 8–9 wt %, etc.). It could provide a guidance for the further design of the new generation of RAFM steels with better comprehensive properties.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jnucmat.2019.151823.

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