

WELDING WIRE COMPOSITION DESIGN FOR A514 HIGH-STRENGTH STEEL WELDED JOINTS BASED ON AN INTERPRETABLE RANDOM FOREST MODEL

METODA NAČRTOVANJA KEMIJSKE SESTAVE VARILNE ŽICE ZA ZVARNI SPOJ IZ JEKLA Z VISOKO TRDNOSTJO TIPA A514 NA PODLAGI RAZLOŽLJIVEGA MODELA NAKLJUČNEGA GOZDA

Dinglu Wu, Yutong Zhao, Feiyang Tao, Jiasong Zhang, Bowen Song, Zhifeng Yan,
Wenxian Wang*

College of Materials Science and Engineering, Taiyuan University of Technology, Taiyuan 030024, China

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To address the challenge of designing welding wire compositions for high-strength steel, this study constructs a random forest model based on 119 sets of MAG welding solid wire data. Nine elements, including C and Mn, were used as input features, and four mechanical properties, including tensile strength, were used as output targets. Following five-fold cross-validation to optimise the model hyperparameters, high prediction accuracy was achieved for both the training and test sets. For example, the tensile-strength model achieved a training-set R^2 of 0.905 and a test-set MAPE of 5.782 %. Considering the inherent physical scatter in impact energy at -40°C , a high-reliability Random Forest classification model (Threshold=100 J) was innovatively developed to ensure design safety, achieving a test accuracy of 79.17 % and an AUC of 0.844. SHAP and partial dependence plot analyses showed that Mo, Ni, and Mn are positively correlated with tensile strength and yield strength, while Cr, Si, P, etc., are negatively correlated with elongation after fracture and significantly decrease the probability of achieving high impact toughness at low temperatures. To eliminate subjective bias, a high-throughput virtual screening framework combining Latin Hypercube Sampling (LHS) and Mahalanobis distance applicability domain (AD) evaluation was established. Based on rigid multi-objective engineering constraints, the optimal welding wire composition range was quantitatively determined. This data-driven method can effectively shorten the R&D cycle and provides a scientific and quantitative basis for wire composition design.

Keywords: high-strength steel welded joint; random forest; mechanical property prediction; model optimization; wire design

V članku avtorji opisujejo študijo, ki se osredotoča na zahtevno načrtovanje kemijske sestave varilne žice za jeklo z visoko trdnostjo tipa A514. Avtorji so konstruirali model naključnega gozda, ki je temeljil na 119-tih nizih podatkov o varilni žici za varjenje z MAG postopkom (angl.: Metal Active Gas welding). Kot vhodne parametre so izbrali devet (9) glavnih kemijskih elementov in za izhodne cilje štiri (4) glavne mehanske lastnosti, vključno z natezno trdnostjo. S 5-kratno navzkrižno validacijo za optimizacijo hiperparametrov modela so avtorji dosegli izjemno natančnost napovedi učnega in testnega niza. Na primer, učni niz za natezno trdnost $R^2 = 0.905$ in testni niz MAPE = 5,782 %. Glede na inherentno fizično razpršitev udarne žilavosti pri -40°C so avtorji študije razvili inovativni visoko zanesljivi klasifikacijski model naključnega gozda (prag =100 J), ki zagotavlja varno načrtovanje in dosega natančnost testa 79,17 % in AUC 0,844. Z uporabo SHAP in analize grafov delnih odvisnosti so ugotovili, da Mo, Ni in Mn kažejo pozitivno korelacijo z natezno trdnostjo in mejo tečenja, medtem ko Cr, Si, P in ostali elementi kažejo negativno korelacijo z raztežkom po lomu in znatno zmanjšajo verjetnost doseganja visoke udarne žilavosti pri nizkih temperaturah. Za odpravo subjektivne pristranskosti so avtorji razvili visokozmogljivo ogrodje za virtualno presejanje, ki združuje vzorčenje latinske hiperkocke (LHS) in vrednotenje domene uporabnosti Mahalanobisove razdalje (AD). Na podlagi togih večciljnih inženirskih omejitev so avtorji kvantitativno določil optimalni razpon kemijske sestave žice. Razvita metoda, ki temelji na realnih podatkih, učinkovito skrajša cikel raziskav in razvoja ter zagotavlja znanstveno in kvantitativno osnovo za načrtovanje sestave žice.

Ključne besede: zvarni spoj iz jekla z visoko trdnostjo, naključni gozd, napovedovanje mehanskih lastnosti, optimizacija modela, načrtovanje kemijske sestave žice

1 INTRODUCTION

High-strength steel has a wide range of applications in modern industry due to its good plasticity, toughness, and workability, particularly in construction machinery and structural engineering.¹ The high strength and toughness of these steels enable it to withstand extreme

weather and long-term operation under high loads, and it has good low-temperature impact toughness, wear resistance, and corrosion resistance, extending the service life of equipment.² In the construction field, high-strength steel is used to manufacture structural components for bridges and high-rise buildings to improve the seismic performance and space utilization of the structure. Its good cold-working and welding performance facilitate more convenient and efficient construction.³

The load-bearing performance and service reliability of welded structural parts directly depend on the me-

*Corresponding author's e-mail:
wangwenxian@tyut.edu.cn (Wenxian Wang)



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chanical properties of the joint, which are essentially functions of the welding process parameters.⁴ In engineering practice, manufacturing enterprises usually need to carry out a large number of process qualification tests as a prerequisite for formulating process specifications.⁵ The traditional trial-and-error process development model requires extensive testing resources and has clear disadvantages, including low efficiency and long development cycles. Some researchers have tried to use numerical simulation technology to predict welding quality to guide process optimization,⁶ but this method has three major technical bottlenecks: the complexity of constructing computational models, long computational times, and demanding hardware requirements;⁷ at the same time, numerical simulation, as a multidisciplinary field, requires practitioners to have expertise in materials science, thermodynamics, and computational science, which greatly limits its widespread industrial application.⁸

The introduction of machine learning technology has opened a new avenue for welding process design.⁹ Manufacturing enterprises have accumulated large amounts of process–performance data in long-term production practice. By building an intelligent analysis system for welding processes to extract value from these data, using algorithms to automatically identify the nonlinear relationship between process parameters and joint performance, and establishing a high-precision prediction model, which can not only realize the quantitative evaluation of joint performance but also provide data-driven decision support for intelligent optimization of process parameters.^{10,11}

At the same time, the mechanical properties of welded joints are not only influenced by welding process parameters but also closely related to the chemical composition of the base metal and welding material. Therefore, establishing the relationship between material composition and mechanical properties is of great significance for optimizing alloy design and improving welding quality.¹² In traditional methods, the optimization of material composition usually relies on empirical formulas, thermodynamic simulation, or a large number of experimental trials, which is costly and time-consuming. In recent years, with the advancement of the Materials Genome Initiative, data-driven composition–performance prediction methods have gradually become a research hotspot.¹³ Machine learning algorithms can mine the complex nonlinear relationship between composition and performance from historical experimental data. For example, Support Vector Regression (SVR) and Random Forest (RF) have been successfully applied to the prediction of alloy strength and ductility.¹⁴

As a major branch of artificial intelligence, machine learning has increasingly been applied across engineering research.¹⁵ In the field of intelligent welding technology, intelligent algorithms such as artificial neural networks (ANNs), support vector machines (SVMs), and genetic algorithms (GAs) have become widely used. It is worth noting that early conventional algorithms have

shown limitations such as insufficient generalization ability and weak robustness in engineering practice, prompting researchers to construct optimized algorithms for specific scenarios through adaptive and iterative improvements. Some scholars have proposed a hybrid architecture strategy, which significantly improves system performance by combining the complementary advantages of different algorithms.¹⁶

Therefore, this study focuses on the design of welding wire compositions for A514 steel used in construction machinery. Based on 119 sets of MAG welding solid-core wire data, a random forest model is constructed to determine the range of wire compositions for welding A514 high-strength steel plate material while satisfying engineering requirements.

2 EXPERIMENTAL EQUIPMENT AND METHODS

2.1 Experimental plan

The base metal used in the experiments was A514 low-alloy high-strength steel, with dimensions of 30 mm × 200 mm × 400 mm. The chemical composition of A514 plate is shown in **Table 1**, and the mechanical properties are shown in **Table 2**.

Table 1: Chemical Composition of A514 Plate (w/%)

Grade	C	Mn	Si	S	P	Cr	Ni	Mo	Cu	Al
A514	0.11	0.99	0.25	0.001	0.01	0.45	1.38	0.53	0.0030	0.027

Table 2: Mechanical Properties of A514 Plate

Grade	σ_b (MPa)	σ_s (MPa)	δ_5 (%)	$A_k(-40\text{ }^\circ\text{C})$ (J)
A514	758	699	26	129

For tensile testing, the specimens were prepared, polished, mounted in the testing machine, and subjected to tensile loading. The composition of the wire and the base metal is determined by ICP-MS, and the samples were analysed after treatment and digestion. Impact-test specimens were prepared according to GB/T 2650-2008, and the test is carried out on a JBW-300W impact testing machine at -40 °C and the fracture surfaces were examined. MAG welding was performed using an OTC/DM500 welding machine, and the AX-MV6 automatic welding robot system is used to complete the welding.

2.2 Random forest

Random forest is a machine-learning algorithm based on ensemble learning, and is a representative bagging-based ensemble method. It generates several different training subsets by bootstrap sampling, and trains a decision tree with each subset. In the process of tree splitting, features are also selected randomly, thus constructing a "forest" containing many decision trees. The final prediction is obtained by aggregating the predic-

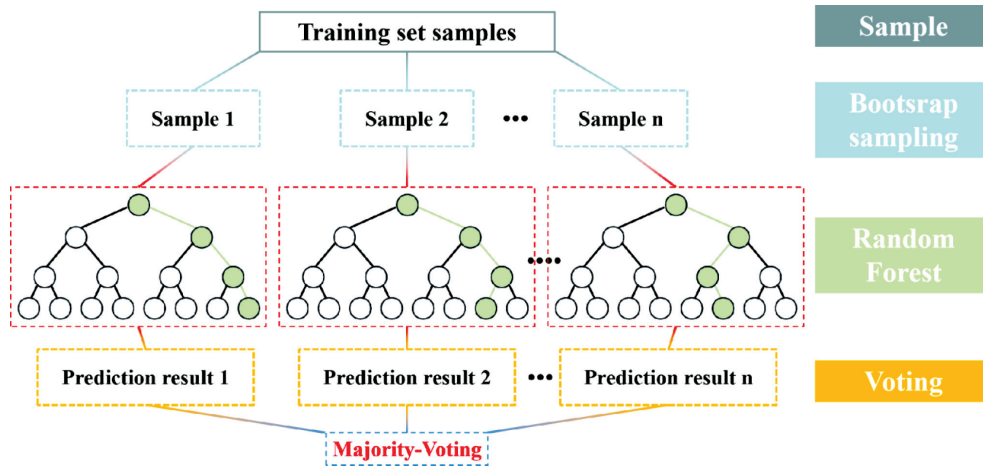


Figure1: Schematic diagram of random forest model

tions of all trees. Its structural schematic diagram is shown in **Figure1**.

The essence of random forest lies in two forms of randomness introduced when training each tree, which ensures that the trees in the forest are diverse and weakly correlated, thus reducing the variance of the whole model.

Randomness 1: Random sampling of data (line sampling)-Bagging

From the original training set, a sample subset (with replacement) is randomly selected by bootstrap sampling. This means: (i) The sample set extracted each time may be the same size as the original set, but the content is different. (ii) Some samples will be drawn repeatedly, while others will not be drawn. Each sampled subset is used to train a decision tree.

Randomness 2: Random selection of features (column sampling)

When each node of the decision tree splits, instead of selecting the optimal split feature from all features, a subset of features is randomly selected first. Then, the best splitting point is only found in this random feature subset. This further increases the diversity among the trees and reduces the dependence of the model on a few strong features.

Without these two sources of randomness, all decision trees trained with the same data set would be almost identical, that is, "homogeneous", and ensemble learning will be meaningless. After introducing randomness, each tree learns based on different data and perspectives, and they make different prediction errors. When many trees make collective decisions, these "mistakes" will cancel each other out, thereby producing more accurate and stable predictions.

To ensure robust model generalisation with the limited dataset (119 samples) and to strike an optimal balance in the bias-variance tradeoff, a comprehensive grid search combined with 5-fold cross-validation was performed. The search spaces for key hyperparameters, as summarized in **Table 3**, were defined based on the physi-

cal characteristics of the target mechanical properties and the risk of overfitting.

For the regression tasks (tensile strength, yield strength, and elongation), a wider search space for the maximum depth (`max_depth`) was used (up to 20) to ensure the models had sufficient complexity to capture highly non-linear metallurgical interactions, such as multi-element solid solution and precipitation strengthening mechanisms. Conversely, for the impact toughness classification task, the search space was deliberately constrained to shallower trees (`max_depth` ranging from 3 to 7) and larger leaf node thresholds (`min_samples_leaf` from 3 to 8). This stringent regularization acts as a crucial mathematical filter to prevent the classifier from memorizing the inherent physical scatter and heterogeneous noise associated with low-temperature impact phenomena. Additionally, the number of decision trees (`n_estimators`) was set to a maximum of 500 to guarantee ensemble stability while avoiding unnecessary computational cost.

Table 3: Super-parameter global optimization space of Random Forest

Hyper-parameters	Regression Task	Classification Task
<code>n_estimators</code>	{50, 100, 500}	{50, 100, 200}
<code>max_depth</code>	{5, 10, 20}	{3, 5, 7}
<code>min_samples_split</code>	{2, 5}	{2, 5}
<code>min_samples_leaf</code>	{1, 3}	{3, 5, 8}

2.3 Model interpretation

The content of each element in the welding wire was treated as an independent input variable. In order to accurately explore its influence on mechanical properties, this study uses partial dependence plots (PDPs) and SHAP (SHapley Additive exPlanations) to quantify the influence of each element.

PDP is a tool used to explain the prediction results of machine learning models. It shows the dependence of the target variable and one or more features while keeping other features unchanged. PDP helps us understand the decision-making process of the model by visualizing the

impact of features on model predictions. Its core idea is to fix the values of certain features and observe how the target variable changes with the change of other features. PDP is generated through the following steps;¹⁹ (i) Select features: select one or more features whose impact on model predictions is to be studied on model predictions. (ii) Fix other features: keep the values of other features unchanged, usually taking their average or median. (iii) Generate predictions: for the selected features, generate a series of values, and calculate the prediction results of the model at each value. (iv) Draw a graph: plot the feature values and the corresponding prediction results to form a PDP.

SHAP is a method derived from cooperative game theory that explains the prediction results (classification and regression) of machine learning models.²⁰ To explain complex machine-learning models, SHAP uses an additive feature attribution method to generate a simplified explanation model. This simplified explanation model $m(\cdot)$ is a linear combination of binary variables, and its definition is expressed by the following formula:²¹

$$m(z') = \Phi_0 + \sum_{i=1}^n z'_i \Phi_i \quad (1)$$

Where $z' \in \{0,1\}$, R represents the coalition vector, Φ_0 is a constant representing the expected value of the prediction, n represents the number of simplified input variables, and Φ_i represents the Shapley value of each input variable. For each input variable, their Shapley values can be calculated by the following formula:²²

$$\Phi_i = \sum_{S \subseteq F \setminus \{i\}} \frac{|S|!(|F|-|S|-1)!}{|F|!} [G_{S \cup \{i\}}(Z_{S \cup \{i\}}) - G_S(Z_S)] \quad (2)$$

In this paper, $G(\cdot)$ represents the random forest, F represents the set of all input variables, and S represents the set of all input variables except i . Therefore, the main advantage of SHAP is that it can provide global or local interpretability analyses of the output of a given prediction model. In addition, SHAP can not only identify globally important features but also quantify the impact of each input variable on the output of the proposed prediction model.

2.4 Model performance evaluation

In order to verify and compare the reliability and effectiveness of the random forest model in predicting the mechanical properties of welded joints, the coefficient of determination (R^2) and the mean absolute percentage error (MAPE) are adopted as the core evaluation criteria in this study. These indicators can comprehensively evaluate the prediction accuracy, generalization ability and stability of the model from complementary perspectives. The formulas for these evaluation metrics are as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y}_i)^2} \quad (3)$$

$$MAPE = \frac{1}{n} \sum_{i=1}^n \frac{|\hat{y}_i - y_i|}{y_i} \times 100\% \quad (4)$$

In the above formula, y_i represents the true value of the sample, $\hat{y}_i$ represents the predicted value obtained from the model, and n is the total number of samples in the data set. $\bar{y}_i$ represents the average value of real sample values.

It should be noted that different modeling strategies were adopted depending on the target mechanical property. Tensile strength, yield strength, and elongation are macroscopic static properties closely related to solid solution strengthening and phase proportions. Therefore, continuous regression models were constructed for these three properties. Conversely, the -40°C impact energy of high-strength steel typically falls within the ductile-brittle transition temperature (DBTT) regime. Its absolute value is intrinsically discrete and highly sensitive to unmodeled microstructural heterogeneities (e.g., trace inclusions, acicular ferrite fractions, and local grain boundary segregation). To avoid severe overfitting caused by applying continuous regression to the limited dataset, the impact toughness prediction was transformed into a high-reliability binary classification task. By setting a stringent engineering safety threshold of 100 J, the model predicts the probability of a composition satisfying high-toughness requirements. For this classification task, Accuracy, Precision, Recall, and the Area Under the Receiver Operating Characteristic Curve (AUC) were adopted as the core evaluation criteria to comprehensively assess the model's generalization ability.

2.5 High-throughput virtual screening and reverse design framework

To overcome the subjectivity of deriving composition ranges solely from qualitative interpretation (such as SHAP and PDP) and to establish a rigorous quantitative mapping between mechanical targets and alloy compositions, a data-driven reverse design framework was constructed. This framework integrates high-throughput virtual screening, Applicability Domain (AD) evaluation, and multi-objective constraint filtering.

First, the Monte Carlo method combined with Latin Hypercube Sampling (LHS) was employed to generate a large number of virtual welding wire compositions. Compared to pseudo-random sampling, LHS is an advanced stratified sampling technique that ensures a more uniform and comprehensive coverage of the high-dimensional composition design space. In this study, 1,000,000 virtual samples were generated within the process-allowable elemental boundaries.

Second, because machine-learning models are inherently interpolative and may produce unreliable predictions when extrapolating, an Applicability Domain (AD) evaluation mechanism based on the Mahalanobis distance was introduced. The Mahalanobis distance accounts for the covariance between different elements and accurately measures the distance from a virtual sample to

Table 4: Partial Data of Training Set

	CHW-40CN	CHW-40Q	CHW-50C2	CHW-50D	CHW-40Cr CuSb	CHW-50A1	CHW-55B2
C	0.075	0.075	0.05	0.08	0.06	0.09	0.075
Mn	1.15	1.13	1.20	1.1	0.53	1.2	1.15
Si	0.5	0.45	0.6	0.55	0.37	0.6	0.68
S	0.008	0.007	0.01	0.01	0.005	0.008	0.009
P	0.013	0.008	0.016	0.01	0.012	0.01	0.013
Cr	0.35	0.35	0	0	0.93	0	1.31
Ni	0.3	0.33	0	0.35	0.19	0.062	0
Cu	0.35	0.25	0.2	0.2	0.43	0.2	0.14
Mo	0	0	0	0	0.015	0.51	0.5
σ_b	525	540	545	520	530	665	646
σ_s	415	430	455	420	430	585	545
δ_5	26	31	26	25	26.5	23	23
A _k (-40 °C)	130	140	60	100	70	55	90

Table 5: Element Composition Range

	C	Mn	Si	S	P	Cr	Ni	Cu	Mo
Maximum	0.32	1.98	0.89	0.017	0.018	8.66	3.62	0.43	1.60
Minimum	0.02	0.50	0.20	0.001	0.001	0.00	0.00	0.00	0.00

the centroid of the original training data. Virtual samples whose Mahalanobis distance exceeded the 99 % confidence interval (P99) of the training set were classified as "out of domain" and excluded, improving the reliability of subsequent predictions.

Finally, the remaining virtual candidates within the AD were evaluated by the trained Random Forest models. By setting rigid multi-objective mechanical constraints based on engineering requirements, candidates that failed to meet the requirements were excluded, and the statistical boundaries of the remaining optimal candidates were extracted to form the final composition design.

3 RESULTS AND DISCUSSION

3.1 MAG Welding Carbon Steel Solid Wire Dataset

A total of 119 datasets for carbon-steel solid wires were collected in this study, and divided into training and test sets at a ratio of 8:2. Nine elements (C, Mn, Si, S, P, Cr, Ni, Cu, and Mo) were used as input parameters, while tensile strength, yield strength, elongation after fracture, and impact energy at -40 °C were used as output parameters. Part of the data is shown in **Table 4**, and the content range of each element in the dataset is shown in **Table 5**.

3.2 The random forest model predicts the composition range of welding wire

3.2.1 Model Evaluation and Tuning

The model-validation process aims to identify the model with the best generalisation performance. The so-called extrapolation performance specifically refers to the prediction efficiency of the prediction system for previously unseen samples, which is a key measure of machine-learning model quality.

This study uses a robust evaluation system, based on a K-fold cross-validation framework. Through the stratified sampling strategy, multiple groups of training-test data pairs are constructed to achieve a reliable estimate of the model's generalization accuracy.

When implementing the K-fold cross-validation framework, this method first performs a random partitioning without replacement on the original training sample set to generate K equal data subgroups. Each iteration cycle selects K-1 subgroups to construct the training domain, and reserves one subgroup as the validation set. After completing K rounds of independent modeling cycles, a corresponding number of base models and their sets of performance metrics are generated. Based on the minimum positioning criterion of the preset optimization objective function, the optimal hyperparameter combination is determined. To account for possible fluctuations in model performance caused by the randomness of data segmentation, this method uses a multi-model performance index integration strategy and evaluates reliability using the mean performance across folds.

As an ensemble learning model, Random Forest improves performance by constructing multiple decision trees and integrating prediction results. Its core mechanism is to use the bootstrap sampling method to generate multiple subsets to train base decision trees, and randomly select feature subsets during node splitting. In Random Forest, the model itself does not need to adjust weight parameters as in a neural network, and its core optimization process focuses on hyperparameter tuning. The hyperparameters to be optimised include the number of base decision trees, the maximum depth of a single tree, the maximum number of features considered during node splitting, the minimum number of samples in leaf nodes, etc. The setting of these hyperparameters directly affects the bias-variance balance of the model: increasing

the number of trees can reduce variance but increase computational cost; depth limitation can prevent overfitting; feature selection strategies affect model diversity.

In practical applications, the K-fold cross-validation method is usually used to tune the hyperparameters of Random Forest. First, define the value range of each hyperparameter, then generate all hyperparameter combinations through the grid search method, perform K-fold cross-validation on each combination, calculate the average performance index such as accuracy for classification problems and mean square error for regression problems, and finally select the hyperparameter combination that produces the best model performance. After determining the optimal hyperparameters, use all training data to retrain the Random Forest model, and use an independent test set that was not used during training to objectively evaluate the final performance of the model.

Table 6: Optimal super-parameter combination of Random Forest

Hyper-parameters	σ_b	σ_s	δ_5	$A_k(-40\text{ }^{\circ}\text{C})$
n_estimators	100	100	500	50
max_depth	10	10	10	5
min_samples_split	2	2	2	2
min_samples_leaf	3	3	3	8

Through the aforementioned grid search process, the optimal hyperparameter combinations for predicting each mechanical property were globally determined, as

summarized in **Table 6**. The results show that the regression models (tensile strength, yield strength, and elongation) achieved optimal performance with a relatively deeper tree structure ($\text{max_depth} = 10$) and smaller leaf nodes ($\text{min_samples_leaf} = 3$), enabling the capture of complex metallurgical interactions. Conversely, the impact toughness classification model converged to a strongly regularised configuration with a shallower tree ($\text{max_depth} = 5$) and larger leaf nodes ($\text{min_samples_leaf} = 8$). This supports the adopted strategy to suppress overfitting on the highly scattered impact data.

As presented in **Table 7**, the optimized Random Forest models demonstrate high prediction accuracy and robust generalization capabilities across all mechanical properties. For the continuous regression tasks, the models achieved high coefficients of determination (R^2) and low Mean Absolute Percentage Errors (MAPE). Specifically, the testing set R^2 values for tensile strength, yield strength, and elongation reached 0.795, 0.810, and 0.7691, respectively, with their corresponding MAPE values all below 7 % (5.782 %, 6.606 % and 6.438 %). As shown in the scatter and line plots of **Figure 2**, the predicted values for these macroscopic static properties closely track the true experimental values. This indicates that the models have successfully captured the complex non-linear metallurgical mapping from elemental compositions to strength and ductility without suffering from severe overfitting.

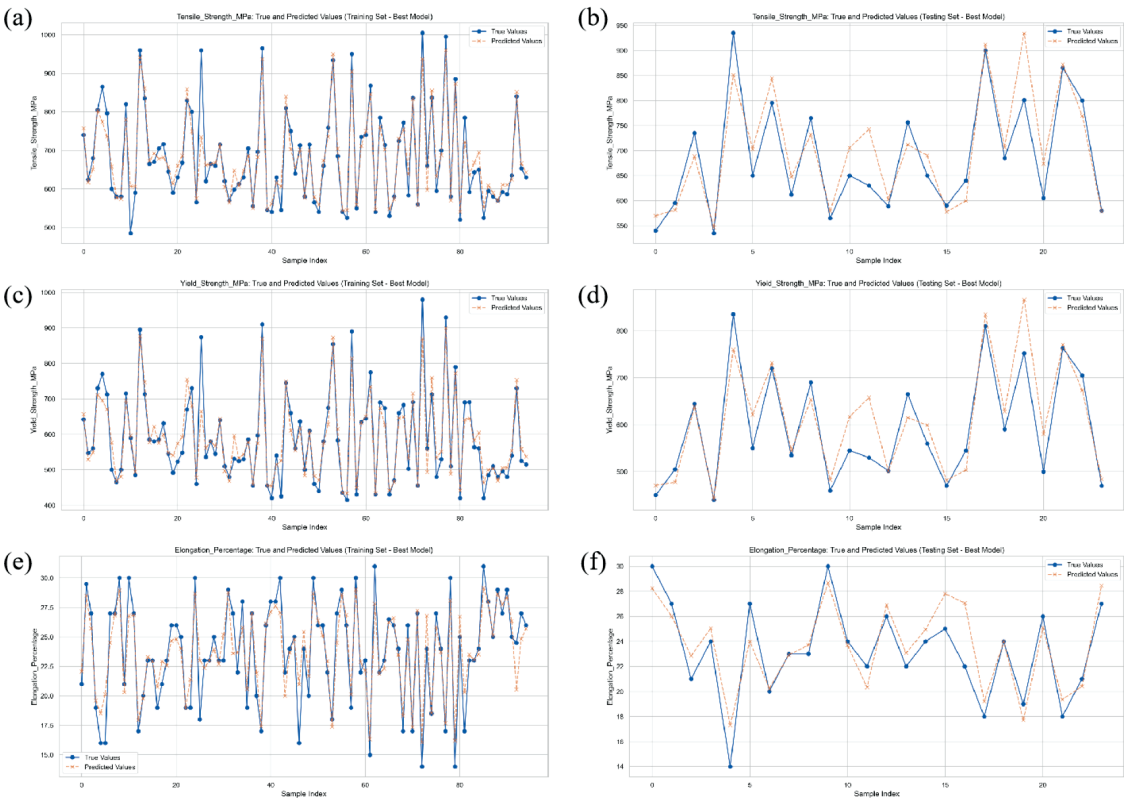


Figure 2: Model prediction accuracy: a) testing set of tensile strength, b) training set of tensile strength, c) testing set of yield strength, d) training set of yield strength, e) testing set of elongation, f) training set of elongation

For the $-40\text{ }^{\circ}\text{C}$ impact toughness, which is highly sensitive to microstructural heterogeneities and exhibits inherent physical scatter, the binary classification model developed in this study (Threshold =100 J) also exhibits good predictive performance. According to **Table 7**, the classification model yielded a testing set F1-score of 0.7095 and an AUC of 0.8444. The ROC curve plotted in **Figure 3a** further confirms the model's strong discriminative ability in distinguishing high-toughness compositions. More importantly, as illustrated by the confusion matrices in **Figure 3b** and **Figure 3c**, the model shows high sensitivity in identifying unqualified samples (the "Fail" class, $< 100\text{ J}$). In the testing set, 13 out of 15 actual low-toughness samples were correctly identified as "Fail". This highly sensitive recognition of substandard compositions is important for engineering applications, as it provides a robust, conservative safety boundary for the subsequent inverse composition design.

Table 7: Random Forest Prediction Accuracy

Objective function	Train set			Test set		
	R^2	MAPE/ %		R^2	MAPE/ %	
σ_b	0.905	3.647		0.795	5.782	
σ_s	0.902	4.724		0.810	6.606	
δ_5	0.856	5.633		0.7691	6.438	
	F1	AUC	Accuracy	F1	AUC	Accuracy
$A_k(-40\text{ }^{\circ}\text{C})$	0.7945	0.9524	0.8421	0.7095	0.8444	0.7917

3.2.2 Model prediction result

3.2.2.1 Welding wire composition and tensile strength

The contribution of each element to tensile strength is shown in **Figure 4**. **Figure 4** shows that among the predicted elements, Mo, Ni, and Mn make the largest contributions to tensile strength, and all are positively correlated.

The partial dependence of tensile strength on Mo content in the range of 0 % to 1.6 % shows an overall stepwise increasing trend. The tensile strength fluctuates slightly at low Mo contents, and the strengthening effect is not significant, with solid solution strengthening dominating. The dependent value rises rapidly in the medium and high content areas, and stabilises at higher contents while remaining at a high level. When the Mo content exceeds 0.19 %, the tensile strength is significantly improved, indicating that precipitation strengthening begins to dominate. At low contents, small amounts of Mo are dissolved in ferrite or austenite, causing lattice distortion and increasing the resistance to dislocation slip, but because its atomic size is similar to that of Fe, the strengthening effect is mild. When the content is high, Mo combines with C to form MC-type or M_2C -type carbides, with a hardness of 1000–1500 HV, which are dispersed within grains and at grain boundaries, hindering dislocation movement and significantly improving strength. Mo also increases the recrystallization temperature, delay dislocation rearrangement and grain growth, maintain a

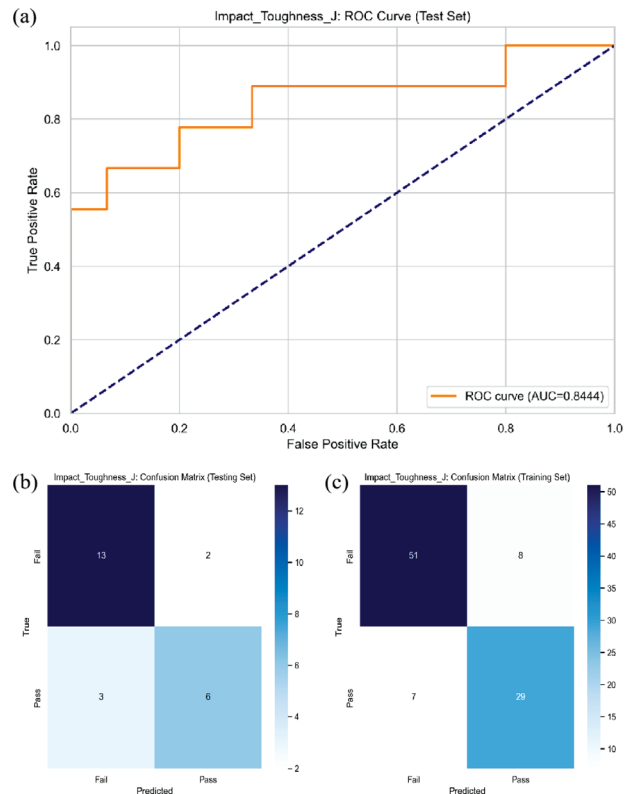


Figure 3: Classification performance of impact toughness model: a) ROC curve of testing set, b) confusion matrix of testing set, c) confusion matrix of training set

high dislocation density, and enhance work hardening ability; and promotes the formation of bainite/martensite and refines the microstructure.

The partial dependence of tensile strength on Ni content in the range of 0 % to 2.6 % continues to rise from 640.09 MPa to 755.42 MPa, showing an approximately linear increase without obvious peaks or inflection points. In the low content area, the tensile strength increases linearly with increasing Ni content, and the strength increases by about 3-5 MPa for every 0.1 % increase in Ni. In the medium and high content areas, the dependent value increases rapidly, reaching 706.92 MPa

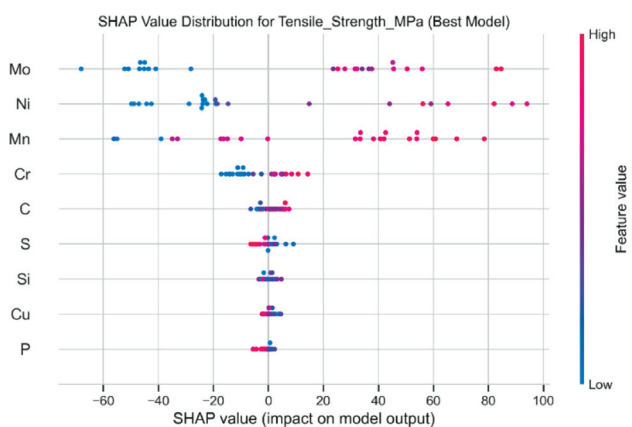


Figure 4: SHAP Plot of Tensile Strength

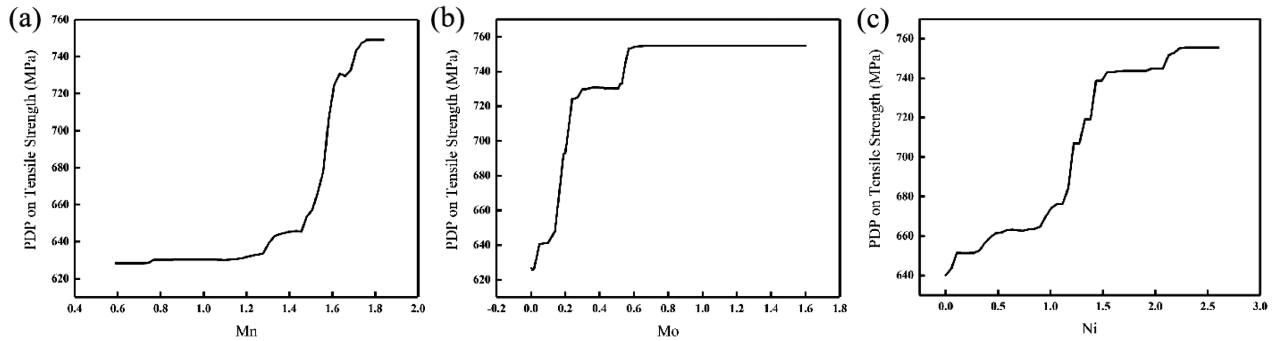


Figure 5: Partial Dependence Plots (PDP) of Tensile Strength: a) PDP of Mn Element, b) PDP of Mo Element, c) PDP of Ni Element

when Ni=1.22 %, and tends to be stable at high content but remains above 750 MPa, with a uniform and continuous strengthening effect. The underlying mechanism is that Ni will expand the γ phase region and reduce the martensitic transformation temperature, so that more austenite is retained at room temperature. Its face-centered cubic structure provides multiple slip systems, increasing the resistance to dislocation movement, and twinning deformation further improves the strength. At the same time, the size difference between Ni atoms and Fe atoms leads to lattice distortion, forming a short-range ordered structure, which hinders dislocation slip; and it does not form harmful brittle phases, thereby improving both strength and toughness.

The partial dependence value of Mn content in the range of 0.59 % to 1.84 % shows a steep, segmented in-

crease. When the content is low, the tensile strength rises slowly, and its strengthening mechanism is mainly solid solution strengthening. The atomic radius of Mn is larger than that of Fe, and when it is solid-dissolved in austenite, it produces strong lattice distortion, and the resistance to dislocation slip is significantly improved. When the content is high, the dependent value rises rapidly, and phase-transformation strengthening then becomes dominant. When the Mn content exceeds 1.3 %, the austenite stabilization effect is significantly enhanced, the proportion of metastable austenite increases, and the work hardening ability is greatly improved.

3.2.2.2 Welding wire composition and yield strength

The contribution of each element to yield strength is shown in **Figure 6**. It can be seen from the image that among the predicted elements, Mn, Ni, and Mo make the largest contributions to yield strength, all of which are positively correlated.

The partial dependence plots are shown in **Figure 7**. Among them, the partial dependence value of molybdenum element yield strength shows a stepwise trend, initially decreasing and then increasing. The strength fluctuates slightly due to the weak solid solution strengthening effect at low content; when the content exceeds 0.1 %, with Mo combining with carbon to form diffusely distributed MC-type or M_2C -type carbides, the precipitation strengthening mechanism dominates, and the strength rises rapidly. Its principal effect is to increase yield strength through carbide-induced inhibition of dislocation slip, refining grains, and inhibiting recrystallization at medium and high contents. The par-

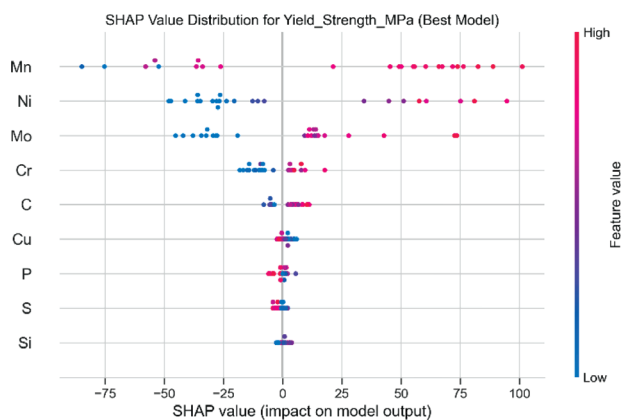


Figure 6: SHAP Plot of Yield Strength

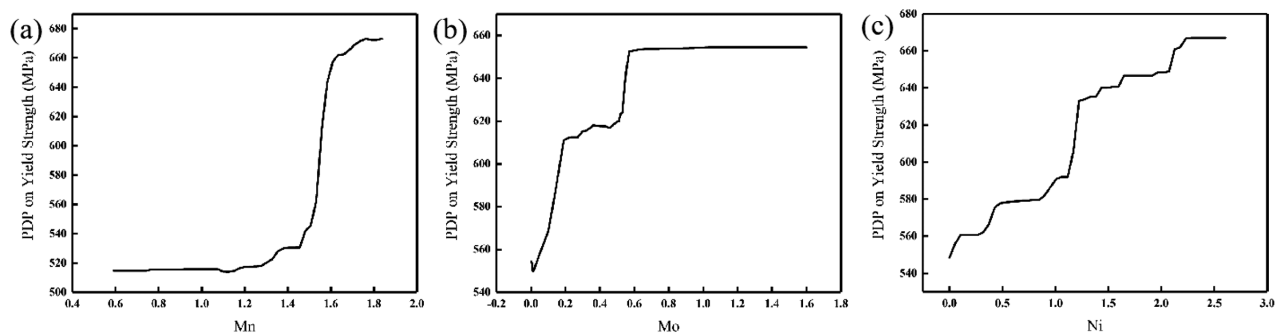


Figure 7: Partial Dependence Plots (PDP) of Yield Strength: a) PDP of Mn Element, b) PDP of Mo Element, c) PDP of Ni Element

tial dependence of yield strength on Ni content shows an accelerating upward trend, and there is no obvious peak in the full content range. At low content, strength increases gradually by solid solution strengthening and austenite stabilization, and at medium and high content, the austenite phase region is expanded to retain more high-strength austenite at room temperature, and the resistance to dislocation slip and work hardening ability are significantly improved. The partial dependence value of manganese element yield strength shows a segmented steep increase. At low content, it is mainly solid solution strengthening. When the content exceeds 1.3 %, the austenite-stabilising effect becomes more pronounced. The metastable austenite undergoes phase transformation-induced plasticity under stress, accompanied by strain-induced martensitic transformation and grain boundary strengthening, and the strength increases rapidly. High Mn forms high-melting-point MnS with sulfur to reduce grain boundary segregation and lower the ferrite transformation temperature to promote a fine-grained microstructure, significantly improving the resistance to dislocation slip.

3.2.2.3 Welding wire composition and elongation after fracture

The contribution of each element to elongation after fracture is shown in **Figure 8**. It can be seen from the image that among the predicted elements, Mn, Mo, and

Cr make the largest contributions to elongation after fracture, and all are negatively correlated with it.

The partial dependence value of Mn content in the range of 0.59–1.84 % gradually decreases, showing an overall decreasing trend. At low Mn contents, Mn, as an austenite-forming element, can expand the austenite phase region, so that the material maintains more austenite with a face-centered cubic structure at room temperature. Austenite has good plastic deformability, and its 12 slip systems provide more paths for dislocation movement, making the material more prone to plastic deformation when stressed, thereby improving elongation. At the same time, when the Mn content is low, Mn segregation at grain boundaries is limited, the grain boundary strength is moderate, and the dislocations easily pass through the grain boundary, reducing crack initiation, which also favours elongation. As the Mn content increases, the partial dependence value decreases significantly. This is because high Mn content promotes the precipitation of hard and brittle phases at the grain boundary, which hinders dislocation movement, making plastic deformation more difficult and reduced elongation. In addition, high Mn content will also reduce the ferrite transformation temperature and prolong the persistence of austenite, which may lead to coarse grains. The total grain boundary area of coarse-grained materials is reduced, the capacity for plastic deformation is reduced, and the elongation is further reduced.

The partial dependence value of Cr element shows a gradual overall decrease, with a more pronounced decrease above 0.24 % Cr. At extremely low contents, the atomic radius of Cr is close to that of Fe, and a small amount is solid-dissolved in ferrite or austenite, producing elastic distortion, which slightly increases the resistance to dislocation slip, but does not significantly reduce plasticity. Even due to the benign effect of solid solution strengthening, it may slightly improve elongation. At the same time, Cr delays carbon diffusion and inhibits pearlite formation, so that the structure is mainly ferrite, maintaining good plasticity. As the Cr content increases, the adverse effects gradually become more pronounced. Cr combines with C to form high-hardness carbides, especially when precipitated at the grain boundary, forming hard particles that act as obstacles. Dislocations need to bypass or cut carbides, consuming

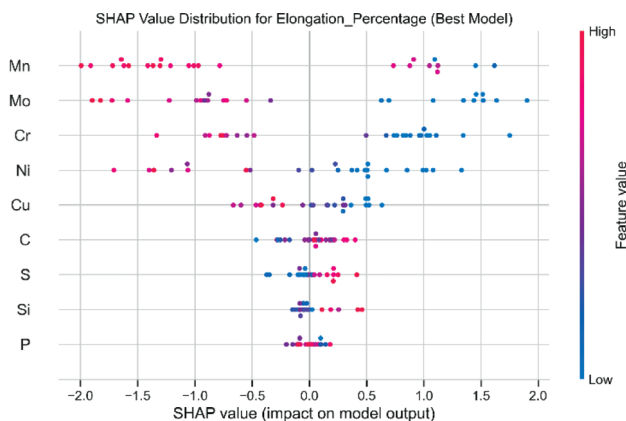


Figure 8: SHAP Plot of Elongation After Fracture

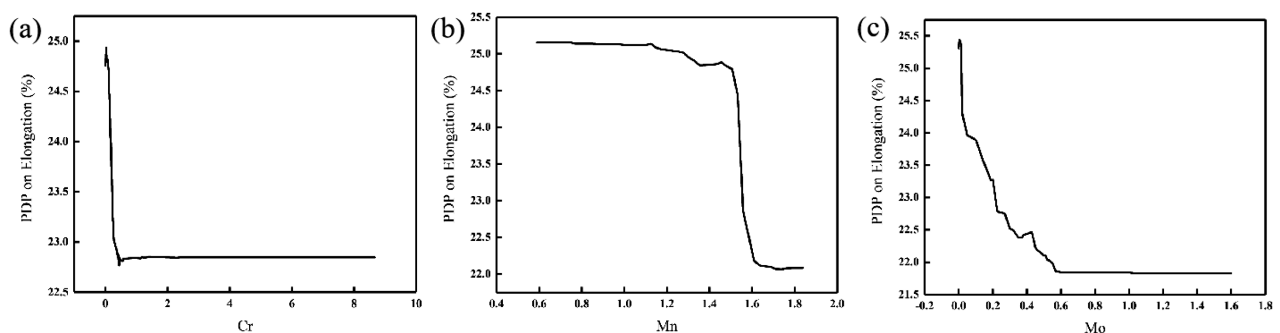


Figure 9: Partial Dependence Plots (PDP) of Elongation: a) PDP of Cr Element, b) PDP of Mn Element, c) PDP of Mo Element

more energy, resulting in a decrease in elongation. Moreover, Cr is a ferrite-forming element. At high contents, δ -ferrite is formed. Although ferrite itself has good plasticity, when coexisting with austenite, the deformation of the two phases is inconsistent, which can produce stress concentrations and reduce the overall plasticity and elongation of the material.

The partial dependence value of Mo element shows a significant decreasing trend, especially after the Mo content is greater than 0.02 %, the rate of decrease accelerates. At extremely low contents, Mo atoms form a Cottrell atmosphere in austenite, pinning dislocations but not completely blocking them, making dislocation movement more uniform, reducing localised deformation, and improving elongation. At the same time, low Mo content delays dislocation rearrangement and maintains work hardening ability, indirectly improving uniform elongation. When the Mo content increases, negative effects begin to dominate. The carbides formed by the combination of Mo and C have extremely high hardness. When distributed in network-like or flake-like morphologies, they seriously hinder dislocation movement, resulting in a sharp drop in elongation. After high-temperature exposure or long-term ageing, Mo also participates in the formation of intermetallic compounds such as γ phase, and these hard and brittle phases significantly reduce plasticity. In addition, Mo segregation at the grain boundary reduces grain-boundary cohesion, especially during the welding cooling process, Mo-enriched regions are prone to liquation cracking, reducing the joint elongation.

3.2.2.4 Welding wire composition and -40°C impact energy

Based on the high-reliability classification model (Threshold ≤ 100 J), the SHAP summary distribution plot (Figure 10) reveals how each element influences the probability of the welding wire achieving excellent low-temperature impact toughness. In this classification context, a negative SHAP value (pushing the model output towards 0) indicates a decreased probability of meeting the 100 J criterion. As shown in the figure, Si, Mo, Cr, and P are the most critical factors, all showing strong negative effects at high concentrations.

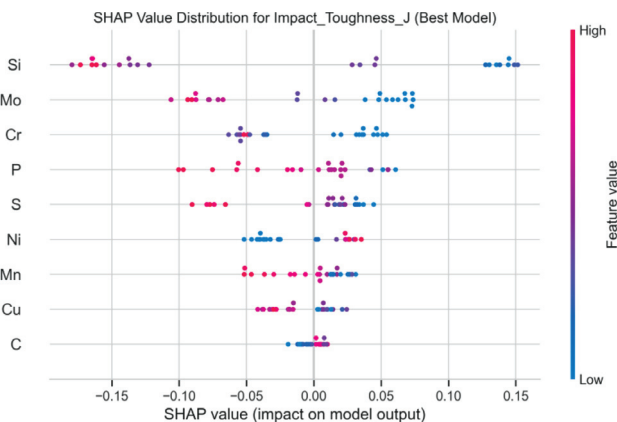


Figure 10: SHAP Plot of Impact Toughness Classification Probability

Si emerges as a highly influential feature. High Si contents produce pronounced negative SHAP values, significantly reducing the pass probability. While an appropriate amount of Si provides solid solution strengthening and deoxidation, excessive Si content leads to the formation of numerous brittle silicide inclusions in the weld metal, which act as primary crack initiation sites. Furthermore, high Si severely deteriorates matrix plasticity, making it difficult for the material to absorb energy through plastic deformation under dynamic impact loads.

Mo and Cr also exhibit strong negative impacts on toughness probability at higher concentrations. Although trace amounts of Mo and Cr refine the microstructure, excessive concentrations strongly promote the precipitation of high-hardness, brittle carbides (such as MC and M_2C types). These hard phases disrupt the deformation compatibility between the grain boundary and the matrix, drastically increasing the risk of brittle cleavage fracture at -40°C .

P and S, as typical detrimental impurity elements, show clear negative effects. When the P content exceeds a critical trace limit, severe segregation at grain boundaries occurs. This segregation fundamentally diminishes the cohesive strength of the boundaries, triggering intergranular fracture and cold brittleness, which strongly reduces the likelihood of meeting the 100 J toughness requirement.

Conversely, Ni is one of the few elements showing a positive effect. Higher Ni content tends to generate positive SHAP values, increasing the probability of high toughness. This is because Ni effectively expands the austenite phase region, promotes a tougher matrix microstructure, and enhances the intrinsic low-temperature plasticity of the ferrite lattice without forming brittle carbides.

3.3 Quantitative Composition Design based on High-throughput Virtual Screening

Based on the reverse design framework established in Section 2.5, 1,000,000 virtual welding wire compositions were generated using LHS. After calculating the Mahalanobis distance, virtual samples falling outside the 99 % confidence interval of the original training data distribution were eliminated to avoid unreliable extrapolation. Subsequently, the valid virtual candidates within the applicability domain were evaluated by the optimized Random Forest models. The rigid engineering requirements listed in Table 8 were applied as simultaneous multi-objective filters. Only candidates that met all four constraints were retained.

Table 8: Properties of Deposited Metal of Target Wire

σ_b (MPa)	σ_s (MPa)	δ_5 (%)	$A_k(-40^{\circ}\text{C})$ (J)
≥ 785	≥ 650	≥ 20	≥ 100

The elemental probability density distributions of the surviving optimal candidates are presented in **Figure 11**.

As shown in **Figure 11**, the optimal compositions do not follow a simple uniform or normal distribution, reflecting the complex non-linear synergistic effects among elements required to achieve a favourable combination of mechanical properties. For instance, to ensure high low-temperature impact toughness while maintaining strength, the algorithm strictly limits the Si content below 0.6 w%, with a sharp cutoff at the upper end to prevent the formation of brittle silicide inclusions. Conversely, the distribution of Ni is heavily skewed towards the higher concentration range (1.5–2.5 w%), supporting the preceding SHAP analysis that higher Ni content is crucial for simultaneously improving strength and intrinsic matrix toughness. Similarly, Mo exhibits a distinct peak around 0.6 w%, indicating an optimal balance where precipitation strengthening is maximized without severely deteriorating ductility.

To provide a robust and statistically sound composition range for practical engineering manufacture, the extreme outliers were trimmed. The 5th and 95th percentiles (P5 – P95) of the distributions in **Figure 11** were used to define the final recommended wire composition boundaries. The updated and highly reliable composition design is summarized in **Table 9**.

4 CONCLUSION

Using the random forest model, this paper this study constructed a composition–mechanical-property prediction model, analysed the effects of key elements on the properties of deposited metal, and finally identified a welding wire composition with improved properties. The main conclusions are as follows:

(1) Based on the collected 119 sets of MAG welding solid wire data, using the contents of nine elements, including C, Mn, and Si, as input features, and 4 mechanical properties including tensile strength, yield strength, elongation after fracture, and $-40\text{ }^{\circ}\text{C}$ impact energy as output targets, a Random Forest prediction model is constructed. Following five-fold cross-validation and grid-search optimisation of the hyperparameters, the model shows high prediction accuracy on both the training set and the test set. Among them, the predictive performance for tensile strength ($R^2=0.905$, test set MAPE=5.782 %), yield strength ($R^2=0.902$, test set MAPE=6.606 %), and elongation after fracture ($R^2=0.856$, test set MAPE=6.438 %) was high, providing a reliable quantitative tool for wire composition optimization.

(2) Strength-enhancing elements (positive correlation): Mo, Ni, and Mn are the main elements affecting

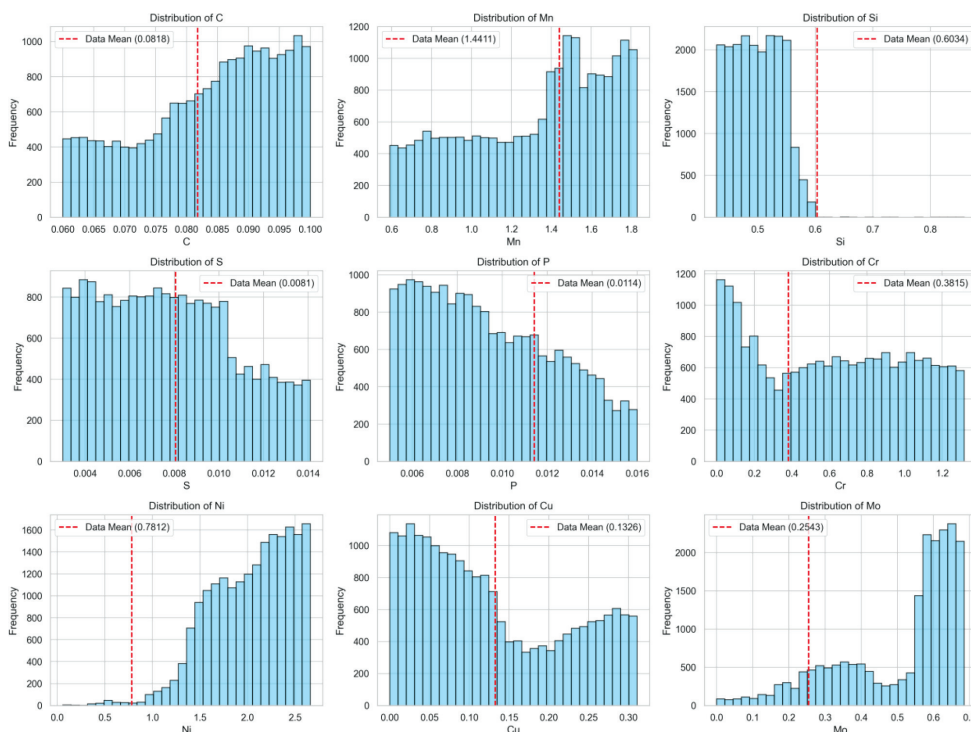


Figure 11: Frequency distributions of elemental compositions for the optimal candidates after high-throughput virtual screening

Table 9: Recommended Welding Wire Composition based on Virtual Screening (w%)

Element	C	Si	Mn	P	S	Cr	Ni	Mo	Cu
Lower Limit	0.063	0.4363	0.6848	0.0054	0.0035	0.0383	1.3313	0.1843	0.0099
Upper Limit	0.0986	0.5629	1.7913	0.0148	0.0131	1.2410	2.6052	0.6737	0.2922

tensile strength and yield strength. Mo improves strength through precipitation strengthening and grain refinement, and the strengthening effect is significant when the content exceeds 0.19 %; Ni improves both strength and toughness by expanding the austenite phase region and solid solution strengthening; Mn significantly improves strength through phase transformation strengthening and grain boundary optimization at medium and high contents (>1.3 %). Toughness-influencing elements (negative correlation): Cr, Si, P, Mn, and Mo negatively affect elongation after fracture and impact energy at -40°C . High contents of Cr and Mo promote the precipitation of hard and brittle phases, hindering dislocation movement; excessive Si leads to silicide inclusions, reducing plasticity; P segregation at grain boundaries significantly reduces low-temperature impact toughness.

(3) To eliminate subjective bias in alloy design, a high-throughput Monte Carlo virtual screening framework combined with Applicability Domain (AD) checking was introduced. By screening 1,000,000 LHS-generated virtual samples against the rigid multi-objective constraints, the optimal composition range was statistically derived. This fully quantitative, data-driven approach not only provides a highly reliable composition range that satisfies the specified strength and toughness requirements, but also provides a quantitative framework for accelerating welding-material R&D.

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