

Supplementary Materials

Integrating physical metallurgy principles and machine learning for predicting continuous cooling phase transformations in steel

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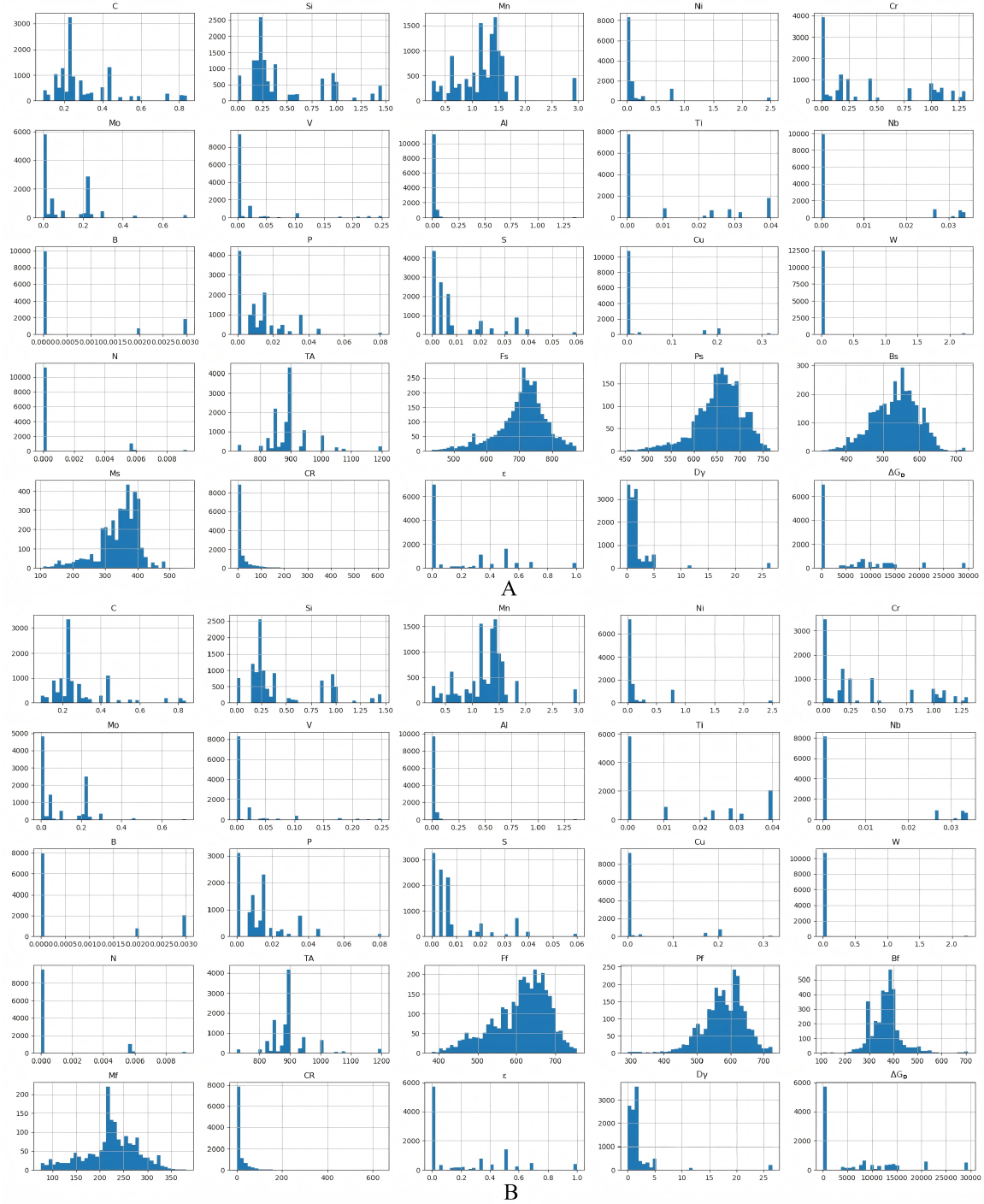
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SM-1: Visualization analysis of each input feature

To intuitively present the data distribution of the database, histograms were plotted to conduct visualization analysis on all input features in this study. **Supplementary Figure 1A and B** show the feature distribution of the phase transformation start temperature and phase transformation finish temperature in the database, respectively.



Supplementary Figure 1. The distribution histograms of feature values in the database. (A) phase transformation start temperature; (B) phase transformation finish temperature. F_s : Ferrite transformation start temperature; P_s : pearlite transformation start temperature; B_s : bainite transformation start temperature; M_s : martensite transformation start temperature; F_f : ferrite transformation finish temperature; P_f : pearlite transformation finish temperature; B_f : bainite transformation finish temperature; M_f : martensite transformation finish temperature; CR: cooling rate; D_γ : austenite grain size; ΔG_D : dislocation energy.

SM-2: Feature selection based on Pearson correlation analysis

To reduce model complexity and improve computational efficiency, the input features of eight sub-databases for phase transformation temperatures were screened prior to model construction. The Pearson correlation coefficient was adopted to evaluate the linear correlation between each feature and the target phase transformation temperature. Features with absolute correlation coefficients below 0.1 were removed, and these discarded features are listed in **Supplementary Table 1**. This procedure effectively removes redundant information and enhances the training efficiency and interpretability of the model.

Supplementary Table 1. Statistics of features filtered out via correlation analysis

Phase Transition Temperature Model	Features Excluded Through Screening
F _s	B, S, W, N
P _s	Al, N
B _s	Mn, S
M _s	Mn, Cr
F _f	Mo, Al
P _f	Ni, Mo, Al
B _f	Al, S, Cu
M _f	Ti, S

F_s: Ferrite transformation start temperature; P_s: pearlite transformation start temperature; B_s: bainite transformation start temperature; M_s: martensite transformation start temperature; F_f: ferrite transformation finish temperature; P_f: pearlite transformation finish temperature; B_f: bainite transformation finish temperature; M_f: martensite transformation finish temperature.

SM-3: Model hyperparameter optimization using grid search and cross validation

In this study, grid search combined with 5-fold cross validation was adopted to systematically optimize model hyperparameters with the objective of minimizing the root mean square error (RMSE). For the random forest (RF) model, the main optimized hyperparameters include the number of decision trees (n_estimators), maximum tree depth (max_depth), etc. For the k-nearest neighbors (K-NN) model, the number of neighbors (n_neighbors) and weight calculation method (weights) were primarily optimized. The optimal parameters of the RF and K-NN models are listed in **Supplementary Tables 2 and 3**, respectively.

Supplementary Table 2. Statistics of optimal parameters selected via grid search for the random forest model

Model	n_estimators	max_ depth	min_samples_ leaf	min_samples_ split	max_ features
F _s	130	30	1	2	log2
P _s	180	30	1	2	log2
B _s	140	20	1	2	log2
M _s	190	30	1	2	log2
F _f	190	30	1	2	log2
P _f	140	30	1	2	log2
B _f	140	30	1	2	log2
M _f	190	20	1	2	log2

n_estimators: number of estimators; max_depth: maximum depth; min_samples_leaf: minimum samples per leaf; min_samples_split: minimum samples required to split an internal node; max_features: maximum number of features.

Supplementary Table 3. Statistics of optimal parameters selected via grid search in the k-nearest neighbors model

Model	n_neighbors	weights
F _s	2	distance
P _s	2	distance
B _s	2	distance
M _s	2	distance
F _f	2	distance
P _f	2	distance
B _f	2	distance
M _f	2	distance

n_neighbors: Number of neighbors.

SM-4: Performance evaluation of random forest model

The coefficient of determination (R^2), mean absolute error (MAE) and root mean square error (RMSE) were adopted to evaluate the prediction performance of the RF model on the test set. According to the quantitative metrics in **Supplementary Table 4**, the R^2 values of the other seven models were at or above 0.99, with the MAE maintained at approximately 3.0 °C, except for the P_s model ($R^2 = 0.977$, MAE = 3.5 °C). Among all models, the M_s model achieved the highest prediction accuracy, with $R^2 = 0.996$ and MAE = 1.9 °C. This phenomenon is attributed to the fact that martensitic transformation is mainly governed by alloying elements, and its characteristics can be easily captured by ensemble learning models.

Supplementary Table 4. Statistics of evaluation metrics in random forest modeling

Model	MAE	RMSE	R^2
F_s	2.7	4.6	0.996
P_s	3.5	7.3	0.977
B_s	3.0	5.9	0.990
M_s	1.9	4.0	0.996
F_f	3.1	5.6	0.994
P_f	3.0	5.7	0.991
B_f	2.6	4.6	0.995
M_f	2.0	2.9	0.997

MAE: Mean absolute error; RMSE: root mean square error; R^2 : coefficient of determination.

SM-5: Performance evaluation of k-nearest neighbor model

The R^2 , and RMSE were used to evaluate the prediction performance of the K-NN model on the test set. The metrics in **Supplementary Table 5** reveal that the P_f model exhibits a large prediction deviation with an RMSE of 14.5 °C, which is probably due to its high sensitivity to local outliers. Nevertheless, it still maintains basic prediction capability with an MAE of 3.5 °C. In addition, the K-NN model delivers slightly better performance than the RF model in the prediction of P_s ($R^2 = 0.980$), demonstrating its advantage in capturing local features.

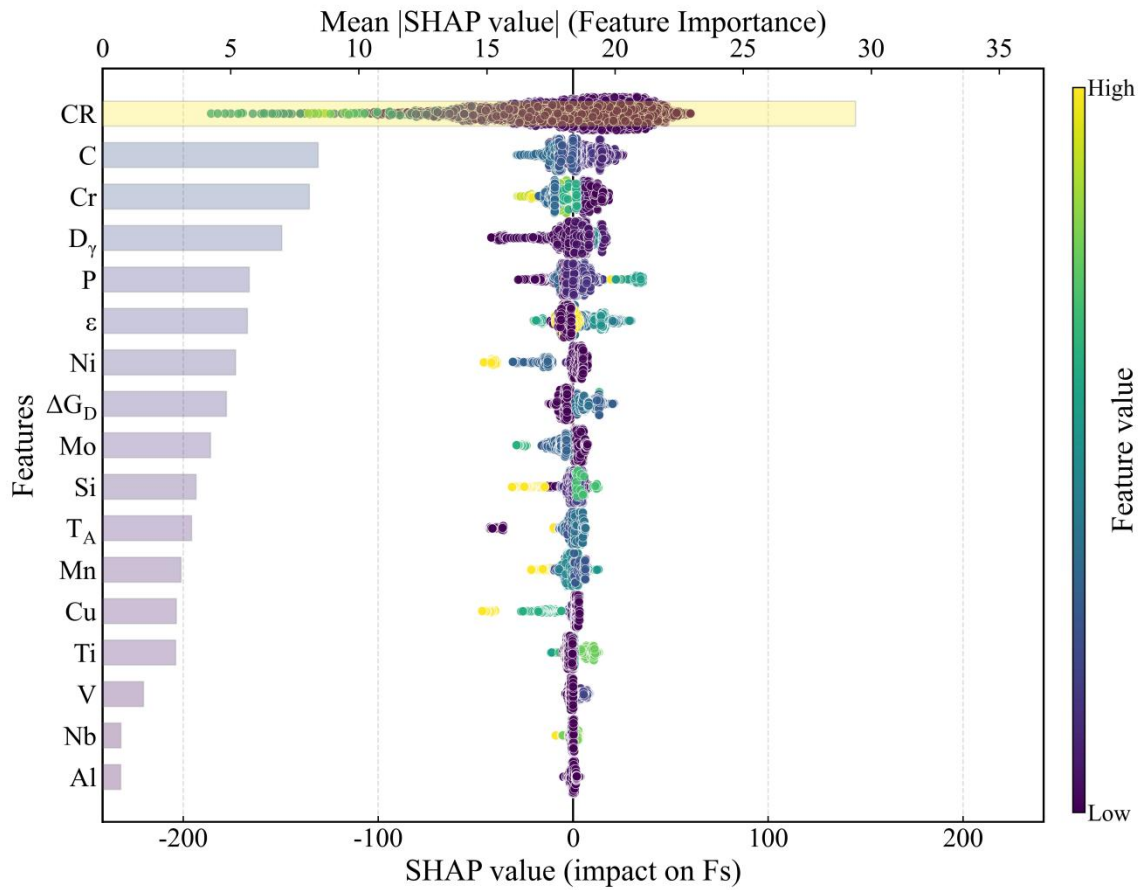
Supplementary Table 5. Statistical summary of evaluation metrics for k-nearest neighbors neighbor modeling

Model	MAE	RMSE	R^2
F_s	2.4	4.1	0.997
P_s	3.2	6.9	0.980
B_s	2.7	5.7	0.991
M_s	1.9	3.8	0.996
F_f	2.5	4.3	0.996
P_f	3.5	14.5	0.943
B_f	2.3	4.3	0.995
M_f	1.8	1.8	0.998

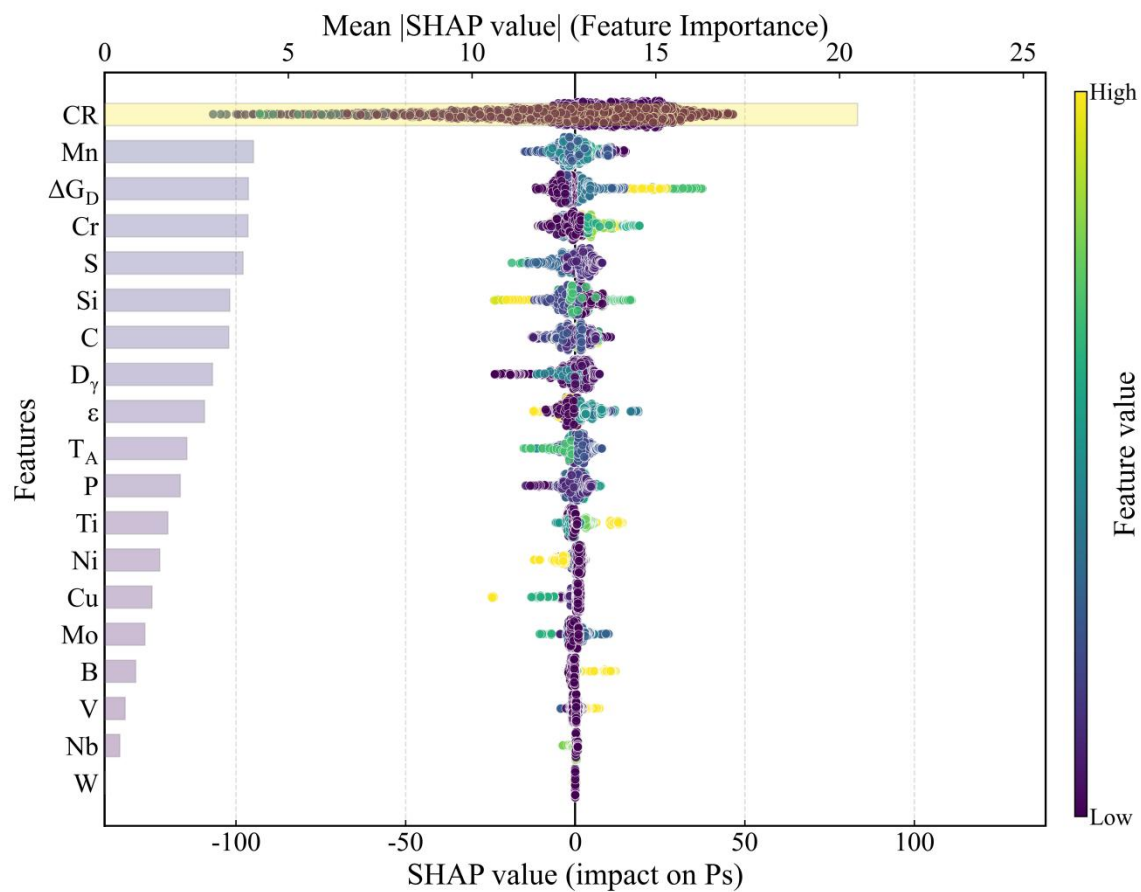
MAE: Mean absolute error; RMSE: root mean square error; R^2 : coefficient of determination.

SM-6: The supplementary compact summary plot (Figure 8) in the main text

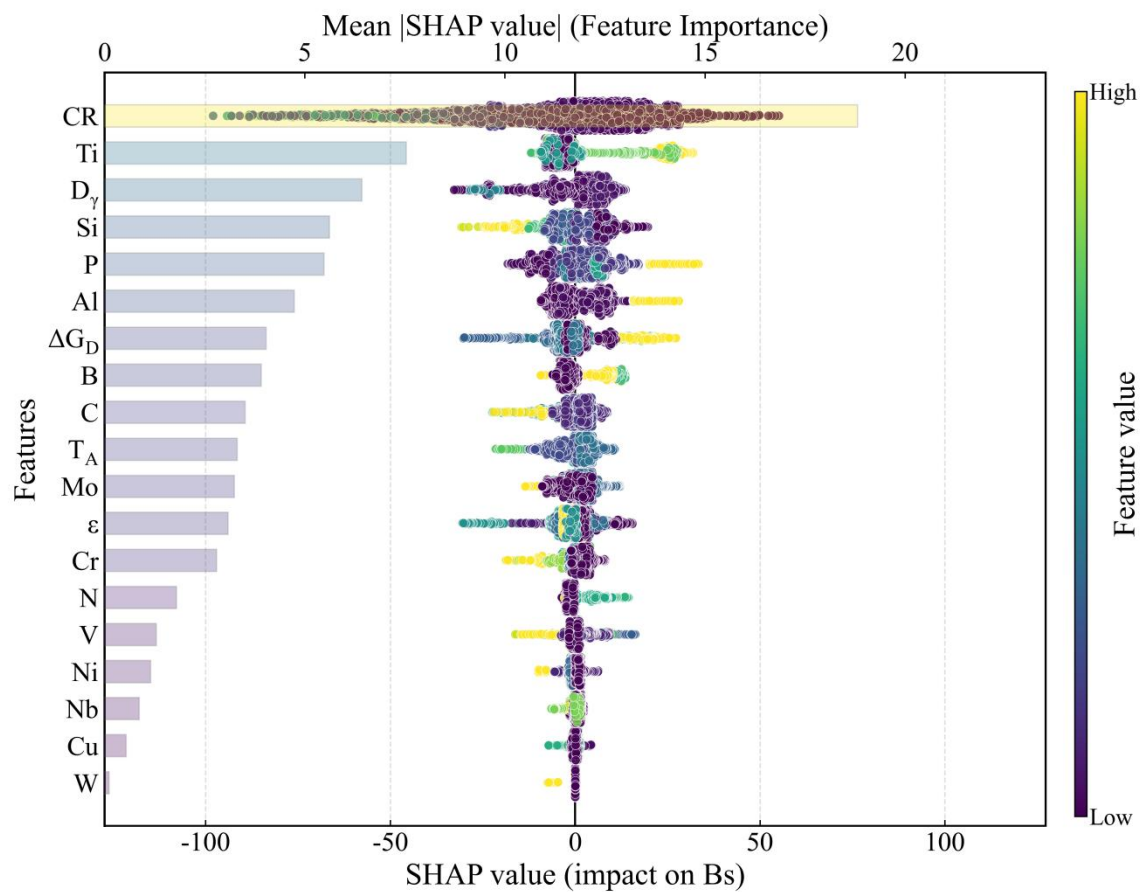
High-resolution individual SHAP summary plots for each of the eight phase transformation temperatures: F_s , P_s , B_s , M_s , F_f , P_f , B_f , and M_f , corresponding to **Figures 8A-H** in the main text. In each plot, features are ranked by SHAP importance from top to bottom. These enlarged individual plots are provided to improve readability and facilitate detailed inspection of feature contributions for each transformation temperature.



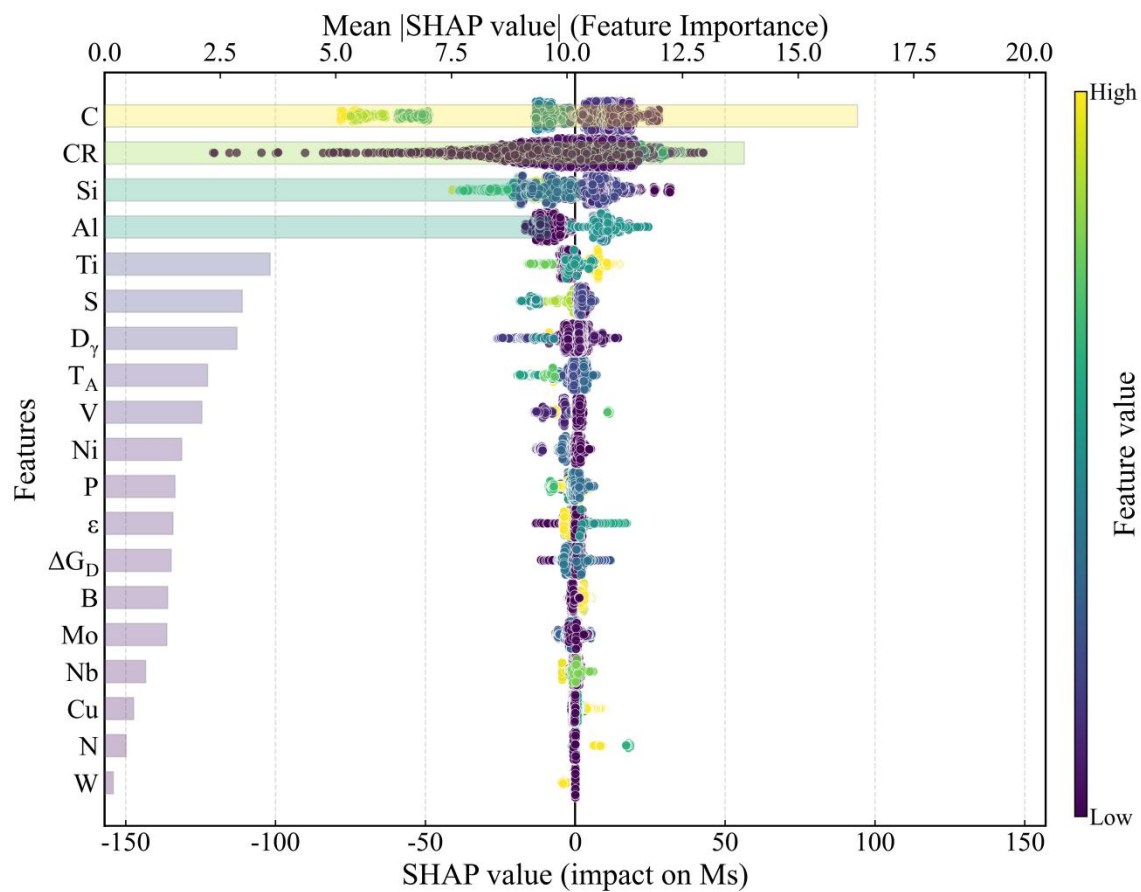
Supplementary Figure 2. SHAP summary plot for ferrite transformation start temperature



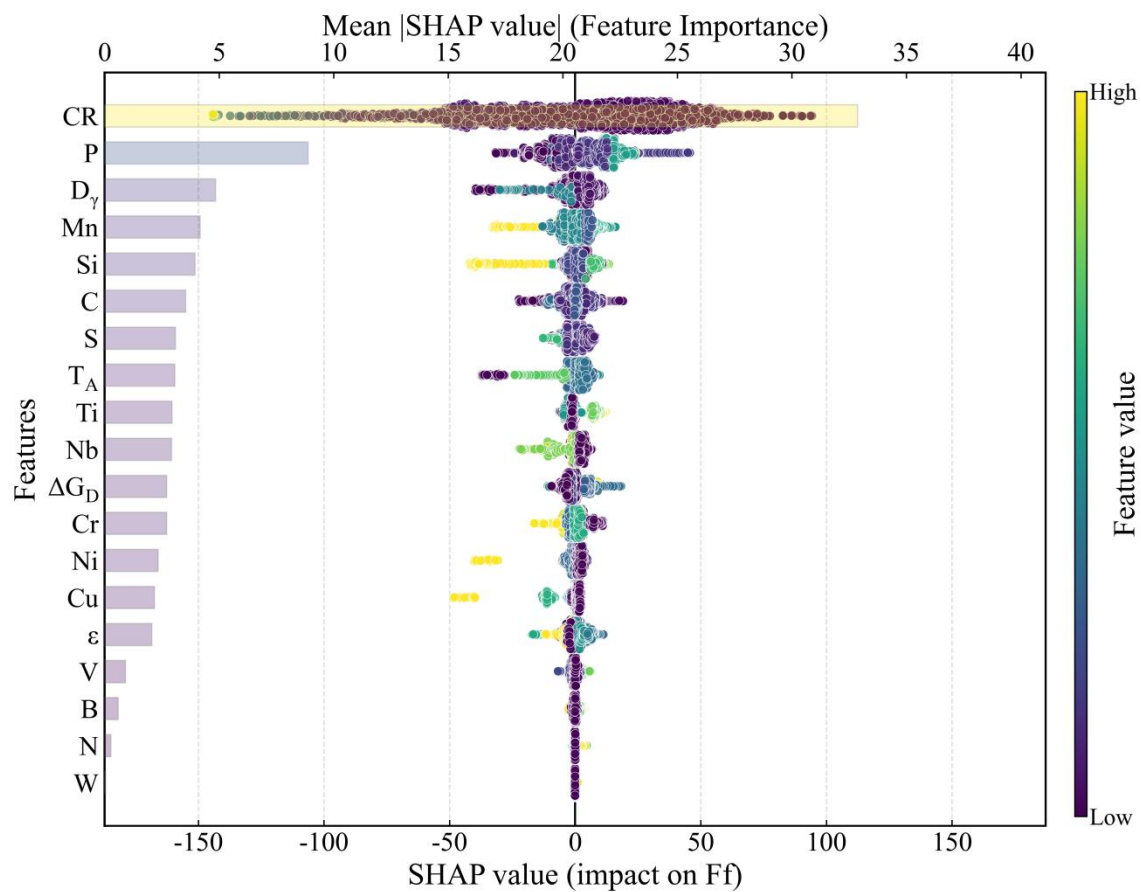
Supplementary Figure 3. SHAP summary plot for pearlite transformation start temperature



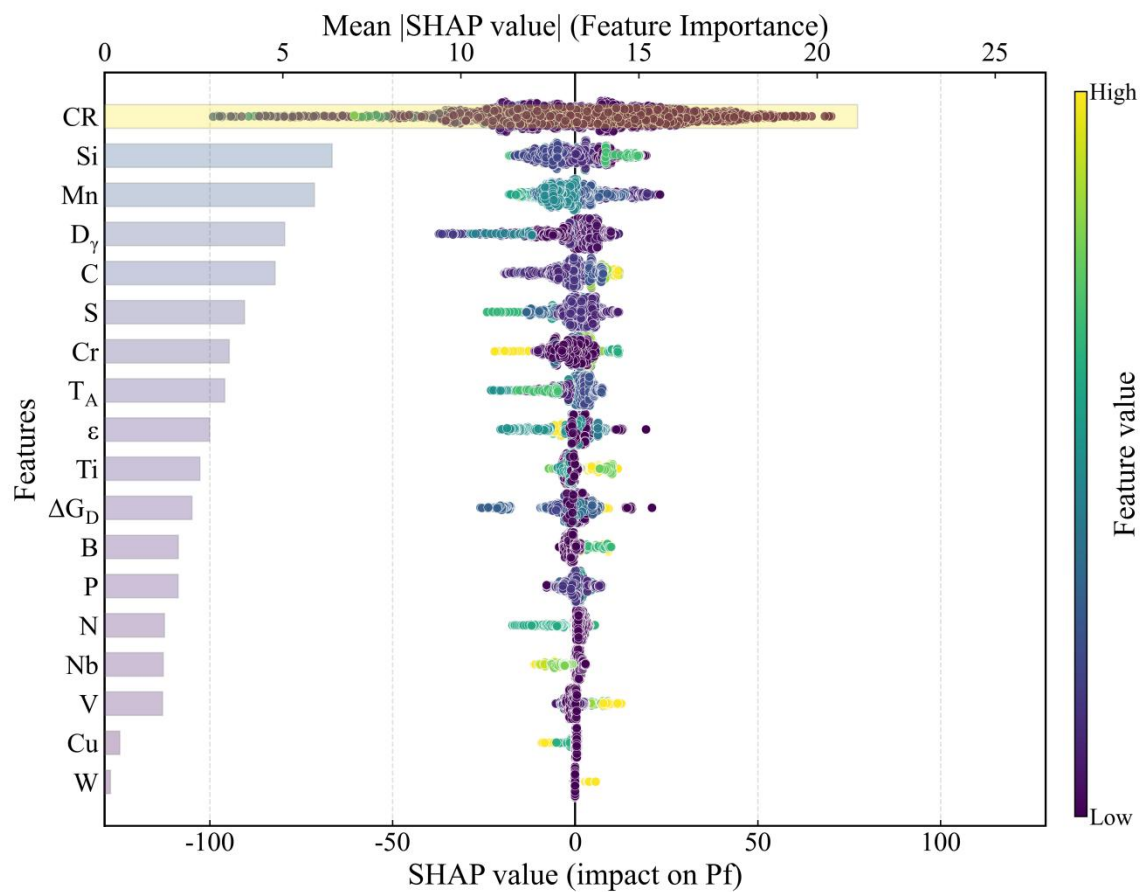
Supplementary Figure 4. SHAP summary plot for bainite transformation start temperature



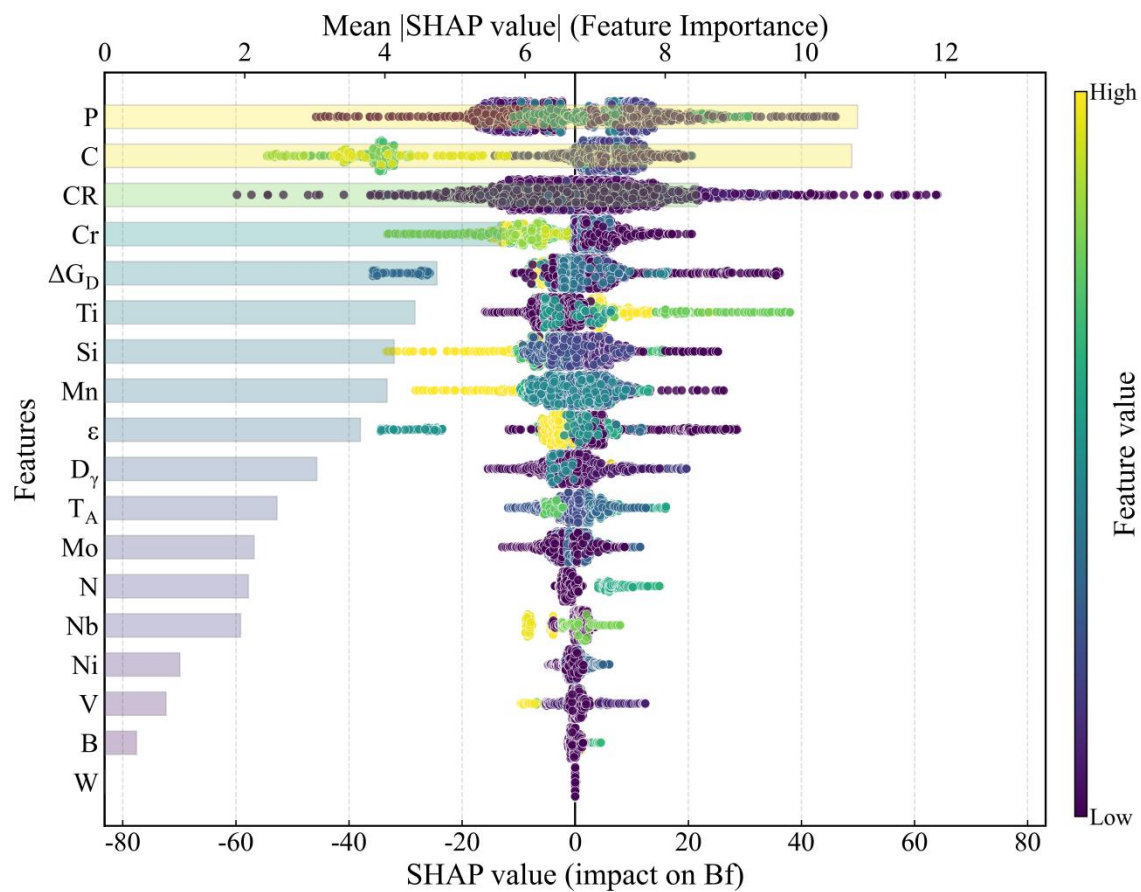
Supplementary Figure 5. SHAP summary plot for martensite transformation start temperature



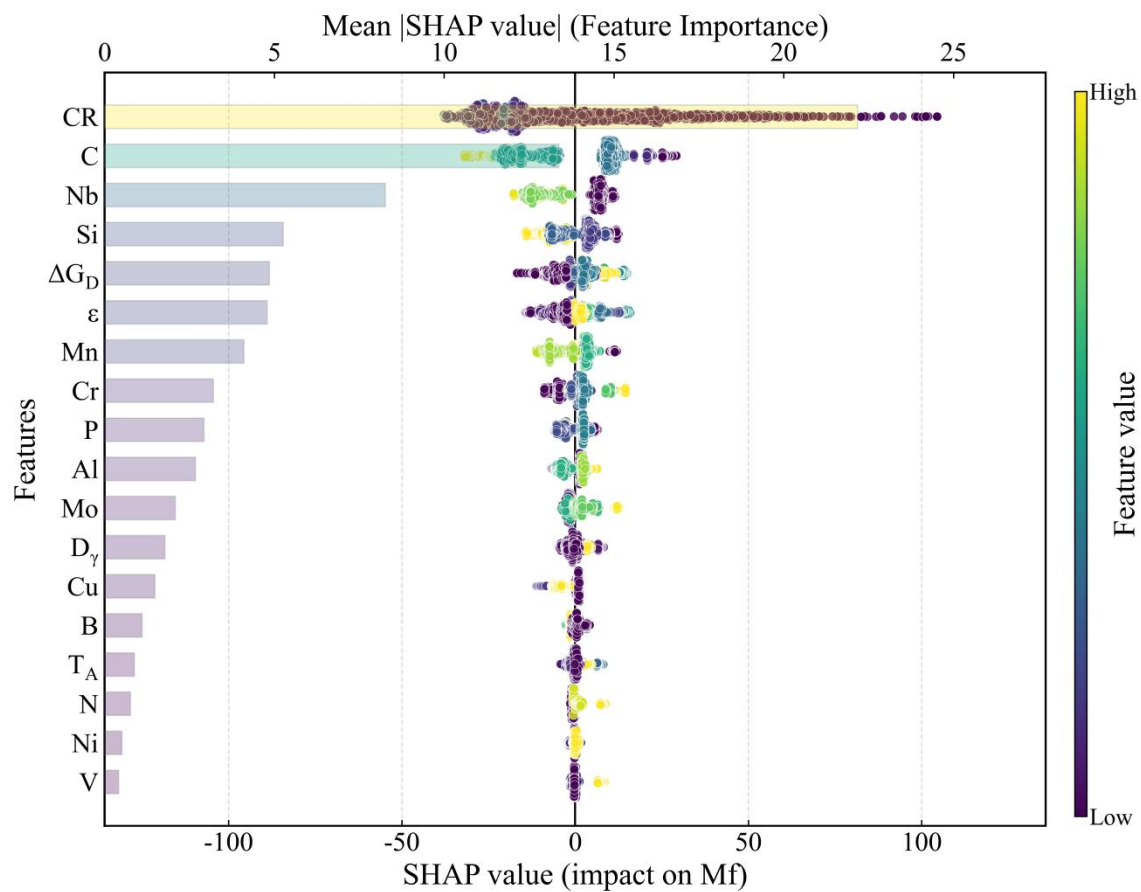
Supplementary Figure 6. SHAP summary plot for ferrite transformation finish temperature



Supplementary Figure 7. SHAP summary plot for pearlite transformation finish temperature



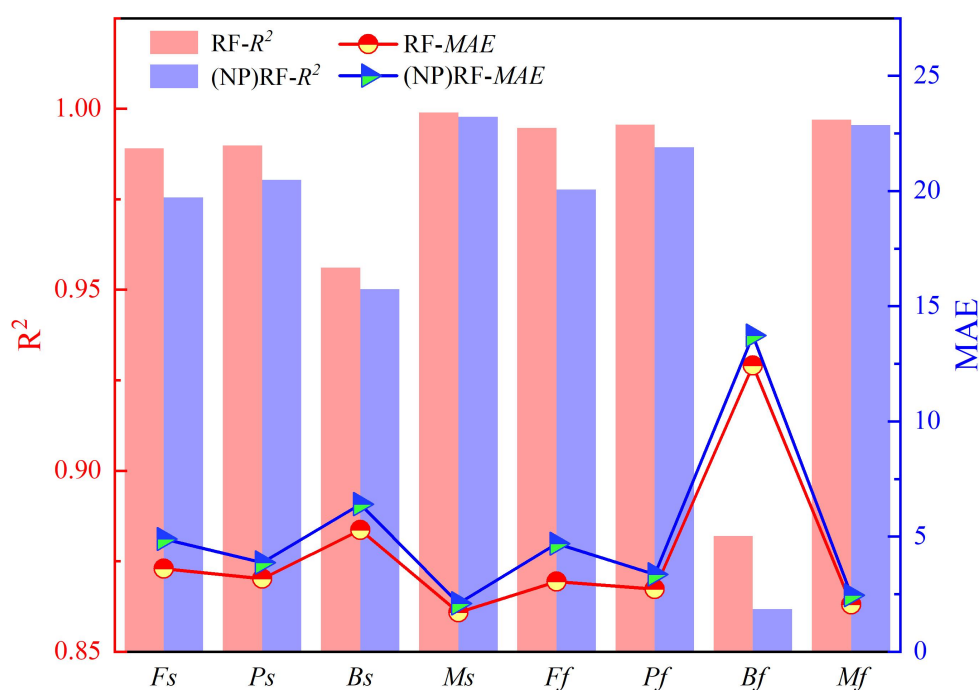
Supplementary Figure 8. SHAP summary plot for bainite transformation finish temperature



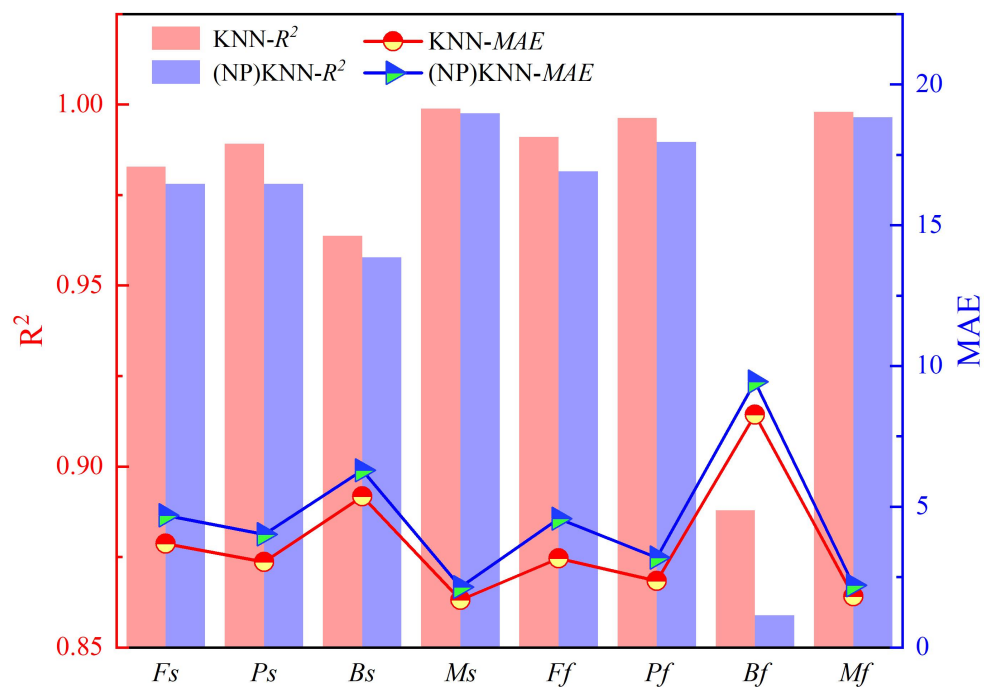
Supplementary Figure 9. SHAP summary plot for martensite transformation finish temperature

SM-7: Performance evaluation of k-nearest neighbor model

To further quantify the contribution of the PM-derived features, we compared model performance with and without ΔG_D and D_γ as inputs. As shown in **Supplementary Figure 2 and 3**, adding these two features consistently improves R^2 and reduces MAE for most transformation temperatures across both RF and K-NN models. This confirms that the PM-guided feature engineering enhances predictive accuracy beyond the baseline composition and thermal parameters.



Supplementary Figure 10. Comparison of RF model performance with and without PM-derived features (ΔG_D and D_γ) across eight transformation temperatures. NP:without PM-derived features.



Supplementary Figure 11. Comparison of K-NN model performance with and without PM-derived features (ΔG_D and D_γ) across eight transformation temperatures. NP:without PM-derived features.