**Journal of Computer Science and Electrical Engineering**
**Print ISSN: 2663-1938**
**Online ISSN: 2663-1946**
**DOI: https://doi.org/10.61784/jcsee3091**

# MACHINE LEARNING-ENHANCED PREDICTION OF PHASE FORMATION IN ALUMINUM-CONTAINING HIGH-ENTROPY ALLOYS: A COMPREHENSIVE STUDY WITH INTERPRETABLE FEATURE ANALYSIS

Lei Zhang
*School of Traffic Management Engineering, Guangxi Police College, Nanning 530028, Guangxi, China.*
*Corresponding Email: zhangleigxec@foxmail.com*

**Abstract:** The phase formation behavior of high-entropy alloys plays a decisive role in their mechanical, thermal, and chemical properties. This paper proposes an interpretable machine learning framework for predicting the phase formation of aluminum-containing HEAs. A dataset of 2256 alloy data points was constructed, covering three phase structures: body-centered cubic (BCC), face-centered cubic (FCC), and multiphase. Two gradient boosting models, Extreme Gradient Boosting and Light Gradient Boosting Machine, were used for multi-class prediction. The model performance was evaluated using learning curves, accuracy, and F1-score using a five-fold cross-validation approach. The results show that the two models have similar prediction accuracy, with Extreme Gradient Boosting performing better with small sample sizes, while Light Gradient Boosting Machine exhibits stronger convergence stability with large sample sizes. To improve model interpretability, the SHAP interpretability method was introduced to quantify the contributions of different descriptors. The results show that the BCC phase is primarily determined by the pure chemical enthalpy Hli and the valence electron concentration VEC; the FCC phase is significantly influenced by VEC, atomic number AN, melting point Tm, and ionization energy Eion; and the Multiphase is dominated by the mixing entropy Smix and the atomic number difference ΔAN. These findings not only verify existing empirical rules for phase selection in high-entropy alloys, but also reveal the role of aluminum in enhancing lattice distortion and entropy-driven stability. They also demonstrate the effectiveness of combining the interpretable gradient boosting model with SHAP, providing a reliable tool for the accelerated design of high-entropy alloys.
**Keywords:** High-entropy alloys; Phase prediction; Machine learning; SHAP analysis

## 1 INTRODUCTION

High entropy alloys (HEAs) are a class of multi-principal alloys composed of at least five main elements, with the atomic percentage of each element ranging from 5% to 35%. Since this alloy design strategy was proposed in 2004, it has attracted widespread interest from researchers due to its unique multi-principal characteristics, showing excellent mechanical properties, corrosion resistance and high-temperature stability [1]. The multi-principal characteristics of HEAs make them have broad application prospects in aerospace, energy and automotive fields [2]. In particular, Aluminum-containing high entropy alloys (HEAl) can significantly reduce the density of the alloy and improve its high-temperature oxidation resistance due to the light weight and good oxidation resistance of aluminum [3]. Therefore, they have important research value and application potential in high-temperature applications. The phase composition of HEA has a decisive influence on its performance. For example, the solid solution phase (SS) is usually related to the hardness and toughness of the alloy, while the amorphous phase (AM) is related to the elastic modulus and corrosion resistance [4]. Therefore, accurately predicting the phase composition of HEA is crucial to optimizing its performance. However, traditional phase prediction methods, such as first principles (DFT) and computational phase diagrams (CALPHAD), have significant limitations when dealing with multi-principal alloys. The DFT method is computationally expensive and the prediction of phase stability of complex systems is not accurate enough, while the CALPHAD method relies on a complete database and lacks support for high-order phase diagram data of HEAs [3]. In recent years, machine learning (ML) methods have been widely used in materials science, especially in the phase prediction of HEAs. ML methods can quickly screen out materials with specific properties by analyzing large amounts of data and identifying complex patterns and relationships [2]. For example, Zeng et al. proposed a phase selection rule for high entropy alloys by combining CALPHAD calculations and ML methods [5]. However, most existing studies focus on improving prediction accuracy and pay insufficient attention to the interpretability of the model. Shapley Additive exPlanations (SHAP), as an emerging interpretability tool, can quantify the contribution of each feature to the model output and provide a deeper physical mechanism explanation for the ML model [6]. Despite this, the combination of model interpretation and practical application in existing research is still insufficient. Based on this, this paper proposes a phase prediction method for aluminum-containing high-entropy alloys based on interpretable machine learning. By constructing Extreme Gradient Boosting (XGB) and Light Gradient Boosting Machine (LGBM) classification models and combining them with the SHAP method, this method not only improves prediction accuracy but also reveals the influence of key physical characteristics on phase stability. This method balances predictive

© By the Author(s) 2025, under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0).

performance with scientific interpretability, providing theoretical support and application reference for the design and optimization of HEAls.

## 2 METHODS

### 2.1 Data Description

This study constructed a HEAl dataset containing 2256 samples to train an interpretable machine learning model to predict its phase formation behavior. The data comes from previous work [7] and related literature in recent years [8], covering a variety of HEAl systems. Each sample contains the alloy composition and its corresponding phase structure label, which is divided into three categories: face-centered cubic (FCC), body-centered cubic (BCC), and mixed phase Multiphase (multiple phases such as FCC, BCC, amorphous phase, and intermetallic compounds exist at the same time). Among them, there are 832 samples of BCC phase, 421 samples of FCC phase, and 1003 samples of Multiphase phase.
The main descriptors of HEA include multiple thermodynamic physical parameters, including enthalpy, elastic energy, mixing entropy, atomic size difference (δ), melting temperature, valence electron concentration (VEC), valence electron concentration difference (ΔVEC), first ionization energy (Eion), vacancy formation energy, bulk modulus (B), shear modulus (G), atomic number (AN), atomic number difference (ΔAN), atomic volume, etc. The above characteristics have been confirmed to have a significant impact on the formation of HEA phase in many studies [9].

### 2.2 Model Selection

In this study, XGB and LGBM were used as the main classification models to predict the phase formation of HEAl. These models are based on the framework of Gradient Boosting Decision Tree (GBDT), but are optimized to handle the multi-classification problem of phase formation of high entropy alloys (such as FCC, BCC and Multiphase).
The basic principle of XGB is to iteratively construct a decision tree weak learner and minimize the loss function using gradient descent such as cross entropy loss. At the same time, L1 and L2 regularization terms are introduced to prevent overfitting, and the second-order Taylor expansion approximate loss function is used to improve optimization efficiency. At the same time, XGB supports parallel computing and tree pruning strategies, which enables it to perform well in processing high-dimensional features such as thermodynamic parameters δ, VEC, and enthalpy in multiple states of high entropy alloys [10]. LGBM further optimizes XGB and reduces memory usage and computing time through a histogram-based decision tree algorithm and a leaf-wise leaf node priority growth strategy. It also introduces Gradient-based One-Side Sampling (GOSS) and Exclusive Feature Bundling (EFB) technologies to efficiently process sparse data and large-scale datasets.
These models have significant advantages over traditional classification methods. Compared with support vector machines (SVM), XGB and LGBM are more efficient in processing nonlinear relationships and high-dimensional data, and do not require kernel function tuning, avoiding the computational bottleneck of SVM on large datasets [11]. Compared with random forests (RF), they capture stronger feature interactions through the gradient boosting mechanism, while RFs rely on simple average integration and may have weaker generalization capabilities on small sample high-entropy alloy datasets. Compared with standard GBDT, the parallel optimization and regularization of XGB and LGBM increase the training speed by 2-10 times. The addition of aluminum often introduces lattice distortion and changes in phase stability, requiring the model to efficiently process complex features such as atomic radius mismatch and electronegativity difference. The above advantages are more suitable for the phase formation prediction of aluminum-containing HEAs [3].

### 2.3 Evaluation Indicators

Model performance is evaluated using learning curves, accuracy, and F1-score.
The learning curve is used to characterize the performance trend of the model on the training set and validation set as the sample size changes. It can diagnose potential overfitting or underfitting problems and provide a reference for sample expansion [12].
Accuracy is defined as:

$$\text{Accuracy} = (TP + TN) / (TP + TN + FP + FN) \quad (1)$$

Where TP, TN, FP, and FN are true positives, true negatives, false positives, and false negatives, respectively. Accuracy intuitively reflects the overall prediction accuracy, but may overestimate model performance in the case of class imbalance [13].
Therefore, F1-score is introduced as a supplementary indicator, which is defined as:

$$F1 = 2 \times (\text{Precision} \times \text{Recall}) / (\text{Precision} + \text{Recall}) \quad (2)$$

$$\text{Where, Precision} = TP / (TP + FP) \quad (3)$$

$$\text{Recall} = TP / (TP + FN) \quad (4)$$

F1-score takes into account both precision and recall, and is particularly suitable for evaluating the classification performance of minority samples such as FCC, thereby avoiding the bias of Accuracy on imbalanced datasets [13].

### 2.3 SHAP Interpretability Analysis

In order to reveal the model decision-making process, the SHAP method is used for interpretability analysis. SHAP is a Shapley value derived from game theory that quantifies the contribution of each descriptor (such as δ, VEC, enthalpy of various states, Smix) to the classification result. Its core idea is to calculate the average marginal contribution of a feature to the model prediction value in all possible feature combinations. For each sample, the SHAP value calculates the marginal contribution of the feature to the prediction [14]. By analyzing the SHAP value, the physical relationship between the descriptor and the alloy phase can be explained. This method goes beyond the traditional "feature importance" ranking and provides a local explanation for each prediction, which can closely link data-driven ML models with the physical mechanisms of materials science.

## 3 RESULTS AND DISCUSSION

### 3.1 Model Performance Comparison

The standardized thermodynamic data were divided into 70% training set and 30% test set, and 5-fold cross-validation prediction was used to obtain the Accuracy learning curves of the XGB and LGBM models, as shown in Figure 1.

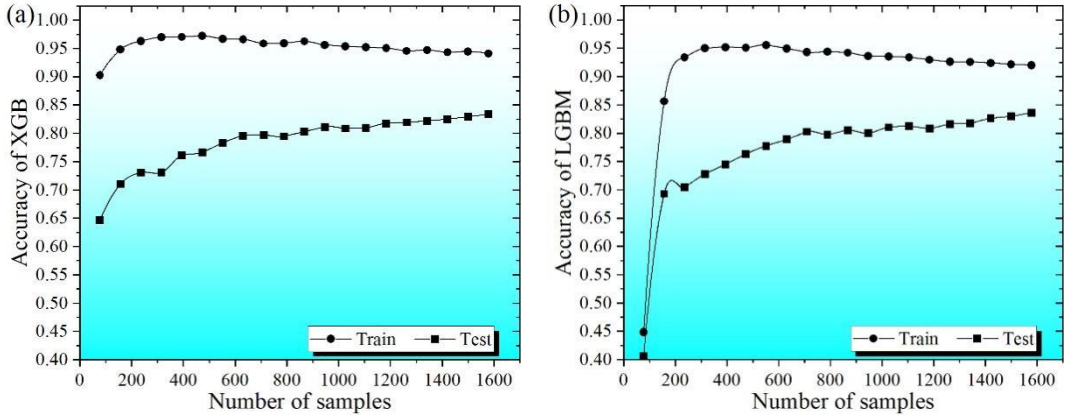


**Figure 1** Accuracy Learning Curves for Different Models

The results show that as the number of samples increases, both models exhibit typical convergence characteristics: training accuracy stabilizes, while test accuracy gradually improves and approaches the training level, indicating good learning and generalization performance. XGB achieves a training accuracy of 0.90 and a test accuracy of 0.64 with 78 samples, indicating a tendency to overfit with small samples. As the number of samples increases, the test accuracy rises to 0.83 (1500-1579 samples), narrowing the gap and converging rapidly, demonstrating its advantages in complex nonlinear modeling. LGBM's training and test accuracy are only 0.44 and 0.41 with 78 samples, reflecting underfitting with small samples. These accuracy increases to 0.95 and 0.73, respectively, with 315 samples. The final test accuracy is 0.836, slightly better than XGB, demonstrating generalization with large samples.

XGB is suitable for modeling small-scale experimental data, while LGBM is more suitable for predictions on high-throughput databases. Accuracy reflects overall accuracy, but because FCC has fewer samples than BCC and Multiphase, class imbalance affects discrimination. To further verify the robustness of the model, the F1-score is introduced as a supplementary metric that more objectively reflects the model's balance in class discrimination.

Figure 2 shows the prediction performance of XGB and LGBM, based on 30 random sampling calculations and the average of the F1-scores for each phase. As can be seen, both models achieve high classification performance across different phase categories, but some differences remain in their detailed performance.

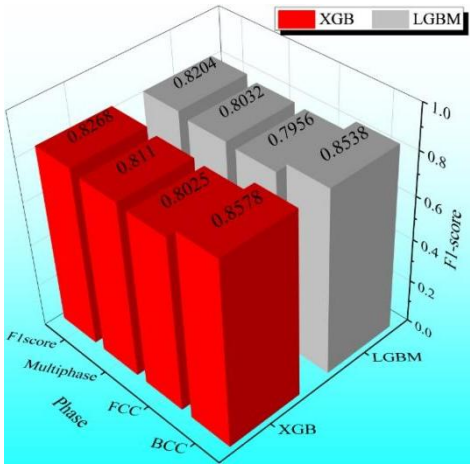


**Figure 2** F1-score of XGB and LGBM in Different Phase Classification Tasks

In the BCC phase classification task, the F1-scores of XGB and LGBM are 0.8578 and 0.8538, respectively. The difference between the two is small, indicating that both models can well capture the characteristic patterns of BCC phase formation. Among them, XGB has a slight advantage, which is related to its layer-by-layer splitting tree structure being more suitable for processing a small number of but strongly correlated features; in the FCC phase, the F1-scores of XGB and LGBM are 0.8025 and 0.7956, respectively, which are lower than the BCC phase as a whole. This difference is largely related to the small number of FCC samples. The limited FCC information in the training set limits the model's discrimination ability in this category, affecting the F1-score; in the Multiphase classification task, the F1-scores of XGB and LGBM are 0.811 and 0.8032, respectively. The model can recognize the laws of Multiphase to a certain extent, but due to its own complexity and ambiguity, the prediction accuracy is still subject to certain limitations; from the weighted F1-score point of view, XGB reaches 0.8268, slightly higher than LGBM's 0.8204, and better than the classification prediction results of the literature [7], indicating that the two perform similarly on this dataset and can provide reliable support for the prediction of high entropy alloy phase formation. XGB is more suitable for phase classification of this dataset as a whole.

In summary, XGB slightly outperforms LGBM in all categories, and is particularly stable in the BCC and FCC phases. However, LGBM's results are very close, and it is more computationally efficient when processing large-scale data.

### 3.2 Interpretability Analysis

To better understand the decision-making process of the XGB and LGBM models in predicting HEAl phase formation, we used SHAP values to analyze the contributions of each descriptor to the BCC, FCC, and Multiphase phases, measuring feature importance based on their absolute values. The SHAP value reflects the marginal contribution of a feature to the predicted output; larger absolute values indicate a more significant impact of the feature on the classification of the corresponding phase. Figure 3 shows the absolute SHAP values of each descriptor's contribution to classification under different models.

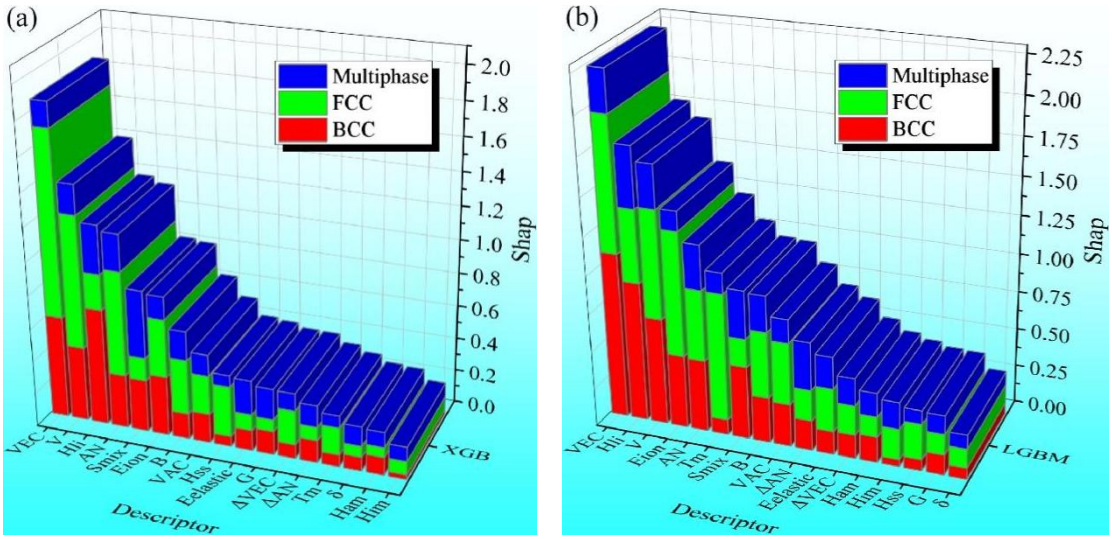


**Figure 3** Contribution of Different Descriptors to BCC, FCC and Multiphase Classification

As can be seen from the figure, for the XGB model, the pure chemical enthalpy Hli and VEC of the BCC phase are the main contributing factors. Hli reflects that the lattice distortion caused by aluminum enhances the stability of the BCC phase, while a low VEC value promotes the formation of the BCC phase [15]. In the FCC phase, VEC is the most dominant, and high VEC drives the FCC structure, followed by V and AN, emphasizing the regulatory role of electron concentration and atomic number on FCC. In the multiphase, Smix is dominant, reflecting that high entropy promotes the coexistence of multiple phases. Hli and elastic energy are also significant, indicating that the pure chemical enthalpy and elastic modulus interact to affect the stability of the multiphase.

For the LGBM model, VEC and Hli are equally critical in the BCC phase. The higher weight of VEC indicates that the LGBM is more dependent on electronic structure, while Hli emphasizes the strengthening effect of aluminum on the BCC. In the FCC phase, Tm and Eion dominate. The melting point and ionization energy reflect the thermodynamic and chemical bonding properties of the FCC phase, with VEC playing a secondary role. In the multiphase, ΔAN and Smix dominate. Atomic number differences and entropic effects drive multiphase formation, with V also contributing.

From the above analysis, it can be seen that XGB is more dependent on VEC and Hli, reflecting its global capture ability of electron concentration and pure chemical enthalpy, which is suitable for the accurate classification of BCC and FCC. LGBM emphasizes Tm and ΔAN, showing its sensitivity to thermodynamic parameters and compositional heterogeneity, and enhancing multiphase prediction. Both models confirm VEC as a key feature, verifying its dominant role in HEA phase selection. Increasing Al increases Hli and ΔAN, tending to BCC or multiphase; regulating VEC can balance the FCC ratio. These findings are consistent with high-throughput data-driven phase prediction studies [16] and provide an interpretable basis for HEA design.

## 4 CONCLUSION

This study constructed an interpretable machine learning framework combining the XGB and LGBM classifiers with SHAP interpretability analysis for phase formation prediction in aluminum-containing high-entropy alloys. Computational results show that XGB converges faster and outperforms LGBM in small sample sizes, while LGBM demonstrates stronger generalization and computational efficiency in large sample sizes. Both models achieved weighted F1-scores exceeding 0.82, outperforming traditional methods. SHAP interpretability analysis revealed that the BCC phase is primarily dependent on pure chemical enthalpy Hli and VEC, while the FCC phase is dominated by VEC and thermodynamic parameters (Tm, Eion), and multiphase formation is controlled by Smix and ΔAN. Aluminum promotes BCC and multiphase formation by increasing pure chemical enthalpy, lattice distortion, and enhancing compositional heterogeneity (ΔAN). VEC further validates its importance as a key metric for HEA phase selection. The interpretable machine learning method proposed in this paper takes into account both predictive performance and physical mechanism explanation. It can not only achieve efficient and scalable phase prediction, but also provide theoretical guidance and data-driven support for the composition design and performance optimization of high-entropy alloys. It can be extended to other complex alloy systems in the future.

## COMPETING INTERESTS

The authors have no relevant financial or non-financial interests to disclose.

## FUNDING

This work is financially supported by the Basic Ability Improvement Project of Young and Middle-aged Teachers in Colleges and Universities of Guangxi Grant (No. 2021KY1938).

## REFERENCES

[1] Yeh J W, Chen S K, Lin S J, et al. Nanostructured high-entropy alloys with multiple principal elements: novel alloy design concepts and outcomes. Advanced Engineering Materials, 2004, 6(5): 299-303.
[2] Li J, Zhang W, Gao Z. Advances in Machine Learning-aided Design of High-entropy Alloys. Materials Reports, 2025, 39(18): 24080091-10.
[3] Yan Y, Hu X, Liao Y, et al. Recent machine learning-driven investigations into high entropy alloys: A comprehensive review. Journal of Alloys and Compounds, 2025, 1010: 177823.
[4] Yu B, Ren Y, Zeng Y, et al. Recent progress in high-entropy alloys: A focused review of preparation processes and properties. Journal of Materials Research and Technology, 2024, 29: 2689-2719.
[5] Zeng Y, Man M, Bai K, et al. Revealing high-fidelity phase selection rules for high entropy alloys: A combined CALPHAD and machine learning study. Materials & design, 2021, 202: 109532.
[6] Karathanasopoulos N, Singh A, Hadjidoukas P. Machine learning-based modelling, feature importance and Shapley additive explanations analysis of variable-stiffness composite beam structures. Structures, Elsevier, 2024, 62: 106206.
[7] Zhang L, Huang J. Efficient Phase Classification in Aluminum-Containing High Entropy Alloys Using Machine Learning. 2024 IEEE First International Conference on Data Intelligence and Innovative Application (DIIA), Nanning, China. 2024, 1-6.
[8] Huang X, Jin C, Zhang C, et al. Machine learning assisted modelling and design of solid solution hardened high entropy alloys. Materials & Design, 2021, 211: 110177.
[9] Wen C, Zhang Y, Wang C, et al. Machine learning assisted design of high entropy alloys with desired property. Acta Materialia, 2019, 170: 109-117.
[10] Chen T, Guestrin C. Xgboost: A scalable tree boosting system. Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining, 2016, 785-794.
[11] Cortes C, Vapnik V. Support-vector networks. Machine learning, 1995, 20(3): 273-297.
[12] Sun Y, Ni J. Machine learning advances in high-entropy alloys: a mini-review. Entropy, 2024, 26(12): 1119.
[13] Sokolova M, Lapalme G. A systematic analysis of performance measures for classification tasks. Information processing & management, 2009, 45(4): 427-437.
[14] Lundberg S M, Lee S I. A unified approach to interpreting model predictions. Proceedings of the 31st International Conference on Neural Information Processing Systems (NIPS'17). Curran Associates Inc., Red Hook, NY, USA, 2017, 4768-4777.
[15] Guo S, Ng C, Lu J, et al. Effect of valence electron concentration on stability of fcc or bcc phase in high entropy alloys. Journal of applied physics, 2011, 109(10): 103505.
[16] Khoa N L, Khanh N D, Quyen H T N, et al. Thermodynamic and Electronic Descriptor-Driven Machine Learning for Phase Prediction in High-Entropy Alloys: Experimental Validation. Journal of Powder Materials, 2025, 32(3): 191-201.