Extended Abstract

Prediction of Elastic Properties in Multi-principal Eelement Alloys Using Machine Learning

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Abstract:

The primary objective of this research is to develop a robust machine-learning framework for the rapid and accurate prediction of elastic properties in multi-principal element alloys (MPEAs), specifically focusing on the Cu–Ni–Au–Pd–Pt system. Given the vast compositional space of MPEAs, traditional first-principles calculations are computationally expensive. This study followed a data-driven approach, employing descriptors such as atomic fractions and binding energy to predict single-crystal elastic constants (C_{11}, C_{12} and C_{44}) and macroscopic moduli (bulk and shear). Various regression models, including Random Forest (RF), Gradient Boosted Decision Trees (GBDT), and Artificial Neural Networks (ANN), were evaluated. The findings demonstrated exceptional predictive accuracy, with R^2 values reaching 0.9989 for the bulk modulus and over 0.96 for individual elastic constants. Binding energy was identified as the most critical descriptor, and SHAP analysis revealed that Platinum (Pt) enhances bulk stiffness while Gold (Au) reduces shear resistance.

Keywords: Multi-principal element alloys; Machine learning; Elastic properties; Binding energy; SHAP analysis.

1. INTRODUCTION

Multi-principal element alloys (MPEAs) have emerged as a significant class of materials due to their exceptional mechanical properties and vast design space. However, predicting their elastic behavior remains a challenge because of the complex chemical interactions between multiple primary elements. While Density Functional Theory (DFT) provides accurate results, its application to high-throughput screening is limited by high computational costs. This study addressed this gap by implementing machine learning (ML) to bridge the gap between chemical composition and mechanical response. Unlike previous studies that focus on simplified systems, this study evaluated the Cu–Ni–Au–Pd–Pt system using a comprehensive set of descriptors. The primary goal was to demonstrate that a compact set of physical descriptors can reproduce elastic constants with high fidelity, offering a faster alternative for materials discovery [1-4].

2. MATERIALS AND METHODS

2.1 .Dataset and Alloy Systems

The dataset was constructed from reported binary-alloy data within the Cu–Ni–Au–Pd–Pt chemical space. The input features included the atomic fractions of the five constituent elements and the binding energy, which served as a proxy for atomic bonding strength.

2.2 .Machine Learning Framework

The study compared several algorithms to capture linear and non-linear relationships:

Tree-based models: GBDT and Random Forest.

Kernel-based and Regularized models: SVR, Lasso, and Ridge regression.

Deep Learning: Artificial Neural Networks (ANN).

Ensemble methods: Stacking models for improved stability.

2.3 .Evaluation Metrics

Models were optimized via hyperparameter tuning and validated using the Coefficient of Determination R^2**,** Mean Absolute Error (MAE), and Root Mean Squared Error (RMSE). To ensure scientific interpretability, SHAP (SHapley Additive exPlanations) analysis was integrated to quantify the influence of each descriptor.

3. RESULTS AND DISCUSSION

3.1. Predictive Performance

The ML models exhibited high precision across all target properties. The bulk modulus was the most accurately predicted (R^2=0.9989, R^2 =0.9989), followed by the shear modulus (R^2=0.9832, R^2 =0.9832). The single-crystal constants C_{11}, $C_{12,}$ and C_{44} also showed strong correlations, with R^2 values of 0.975, 0.964, and 0.963, respectively (see figure 2).

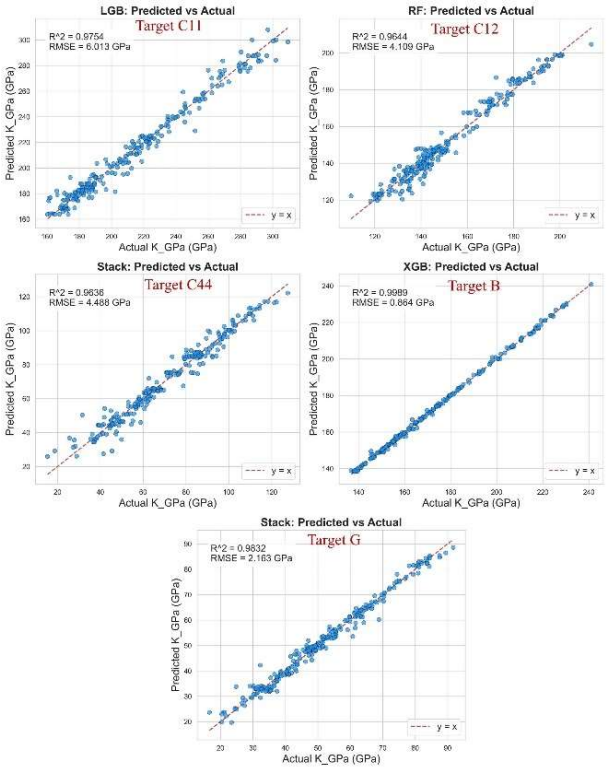
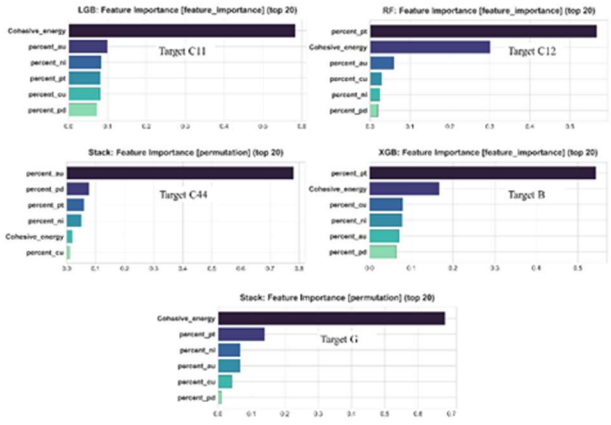


Figure 2: Scatter plots of predicted versus actual values for the target properties.

3.2. Feature Importance and Materials Design

Correlation analysis and SHAP values identified binding energy as the dominant factor governing elastic stiffness. From a materials design perspective, the model indicated that increasing Pt content significantly boosts the bulk modulus, whereas Au content is inversely correlated with shear resistance. These insights allow for the targeted design of alloys with specific mechanical requirements without exhaustive trial-and-error (see figure 3).



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Figure 3. Ranking of the top 20 feature importance in the selected models for the prediction of elastic properties.

4. CONCLUSION

This research demonstrated that machine learning, supported by physically meaningful descriptors like binding energy, offers a highly accurate and efficient route for predicting the elastic properties of MPEAs. The developed models achieved near-perfect correlation for macroscopic moduli and high reliability for individual elastic constants. The integration of SHAP analysis transforms the model from a "black box" into an interpretable design tool. Future work should focus on expanding the dataset to include interstitial elements and evaluating the model's performance under varying temperature and pressure conditions.

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