

Integrating Molecular Dynamics and Machine Learning for Sustainable FeNiCrCoAl High-Entropy Alloys Development

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Abstract. The accelerating global demand for critical minerals, driven by clean energy technologies and climate goals, presents urgent sustainability challenges in materials design. High-entropy alloys (HEAs), particularly FeNiCrCoAl, offer a promising alternative by enabling reduced reliance on critical elements such as Ni, Cr, and Co. This study introduces a data-driven framework that integrates molecular dynamics (MD) simulations with artificial intelligence (AI), specifically machine learning (ML), to predict and optimize the mechanical performance of FeNiCrCoAl HEAs. MD simulations generated over 1800 datasets capturing ultimate tensile strength (UTS) across diverse compositions and temperatures. These data were used to train the Random Forest ML models, achieving high predictive accuracy ($R^2 = 0.975$, RMSE = 0.22). Explainable AI techniques revealed Ni as a key contributor to strength, enabling targeted reduction of Co, Cr, and Al. A novel composition was discovered that reduced critical element content by over 50% achieving nearly double the UTS while retaining more than 90% of its tensile strength across the temperature range. This integrated MD-ML approach provides a scalable and sustainable pathway for alloy design, bridging atomic-scale simulation with predictive modeling to address global resource efficiency goals.

1 Introduction

The swift advancement of civilization has ignited a wave of innovation across diverse industries, particularly in the aerospace, energy, and automotive sectors. These fields demand advanced materials that not only deliver exceptional performance but also exhibit remarkable adaptability to extreme environments. Traditionally, the design of alloys has relied on the incremental addition of a select few base elements. While this approach has proven effective, it imposes limitations on the mechanical performance and versatility of materials [1]. Ni-based superalloys have long reigned supreme in high-temperature structural applications, celebrated for their outstanding strength and thermal stability. Yet, the incorporation of critical elements such as molybdenum, cobalt, and tantalum significantly inflates production costs and raises pressing concerns about long-term sustainability and security of the supply chain. This highlights the urgent need for innovative solutions in materials science to meet the demands of modern industry.

The limitations of traditional materials have sparked the emergence of high-entropy alloys (HEAs), an exciting class of materials comprising five or more principal elements in nearly equal proportions. HEAs are characterized by their high configurational entropy, which enhances the formation of stable solid solution phases while circumventing the pitfalls of brittle intermetallic compounds [2]. This unique thermodynamic behavior, along with their relatively low

density, endows HEAs with extraordinary mechanical properties, including impressive strength, exceptional ductility, remarkable thermal stability, and outstanding resistance to wear and corrosion [3]. Among the most intriguing HEA systems is FeNiCrCoAl, celebrated for its excellent oxidation and corrosion resistance even at elevated temperatures [4]. However, the reliance on critical elements such as Co, combined with the vast compositional landscape these alloys offer, renders experimental optimization both a time-consuming and costly endeavor.

Sustainable alloy design marks a remarkable breakthrough in materials engineering, aiming to revolutionize our approach to reducing environmental impact while simultaneously enhancing mechanical performance and resource efficiency. As depicted in Fig. 1, traditional experimental methods, though essential, often grapple with the burdens of high costs and protracted development cycles due to their trial-and-error nature. To transcend these limitations, innovative computational techniques have emerged as game-changers in the realm of alloy discovery. First-principles calculations yield precise predictions of phase stability and electronic structure, yet they often come with high computational costs and scalability challenges [5]. In contrast, molecular dynamics (MD) simulations provide rich, atomistic insights into mechanical behavior across various loading and thermal conditions. When synergized with machine learning (ML), these simulations formulate predictive models that seamlessly connect composition to mechanical properties,

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drastically minimizing the need for extensive experimental trials [6]. This dynamic integration of MD and ML offers a compelling, data-driven alternative that not only accelerates the discovery of new alloys but also curtails reliance on critical elements and significantly reduces waste [7,8]. This visionary approach directly champions several Sustainable Development Goals (SDGs): SDG 7 (Affordable and Clean Energy) by paving the way for energy-efficient materials in clean technologies; SDG 9 (Industry, Innovation, and Infrastructure) through groundbreaking advancements in computational alloy design and manufacturing; SDG 12 (Responsible Consumption and Production) by endorsing optimized compositions and waste reduction; and SDG 13 (Climate Action) by lowering the carbon footprint tied to material production. By harmonizing atomistic simulations with predictive modeling, researchers are empowered to swiftly explore vast

compositional landscapes, slashing experimental costs and timelines while playing a crucial role in nurturing a sustainable and resilient materials ecosystem.

In this study, we delve into the fascinating world of HEAs with a focus on the FeNiCrCoAl composition. Utilizing cutting-edge MD simulations, we systematically explore their ultimate tensile strength (UTS) across a diverse array of compositions and temperatures. The rich dataset produced from these simulations serves as a foundation for training sophisticated machine learning models, notably the random forest (RF) approach, to predict the mechanical behavior of these alloys and to uncover the most promising compositions. This research builds on the insightful foundations laid by Elgack et al. [7] and Achmad et al. [8], and it contributes significantly to the establishment of a scalable, data-driven framework for the innovative and sustainable HEA design.

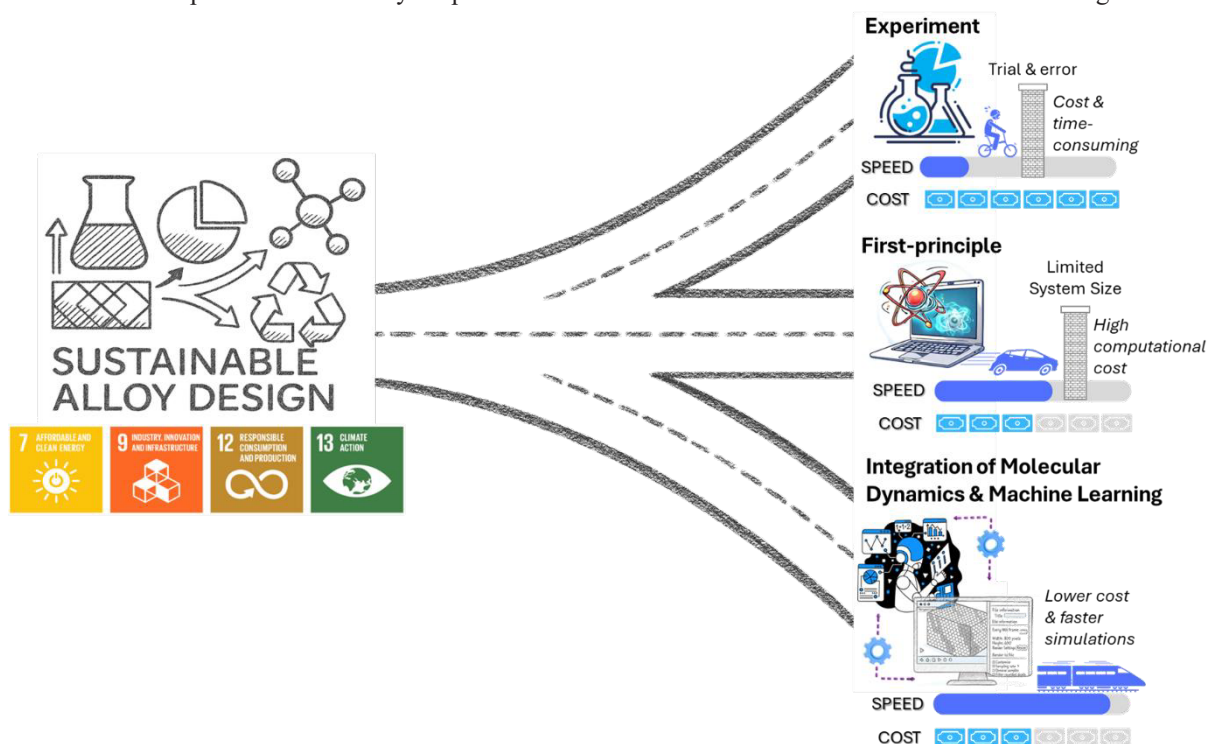


Fig. 1. Comparative overview of alloy design methods highlighting the efficiency and sustainability benefits of integrating molecular dynamics and machine learning over traditional experiments and first-principles calculations.

2 Computational Methodology

The flowsheet in Fig. 2 illustrates the integrated computational methodology used to predict the mechanical properties of FeNiCrCoAl HEAs. The process begins by defining the input parameters, which include simulation settings, alloy composition, and temperature ranges. These inputs are then used in MD simulations, specifically in uniaxial tensile tests conducted with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software. This generates data on tensile strength as a function of both composition and temperature. The resulting data is compiled into a comprehensive UTS database. This dataset is subsequently divided into training (80%) and validation (20%) datasets. Using the Random Forest (RF) ML algorithm, models are trained to understand

the relationships between the input features and mechanical properties. Finally, the trained model is evaluated and used to make UTS predictions.

2.1 Molecular Dynamics Method

The MD simulations employed an interatomic potential specifically developed for Fe–Ni–Cr–Co–Al systems by Farkas and Caro [9], which has been validated for accurately capturing atomic-scale interactions and deformation mechanisms in multi-component alloys. The compositional space was systematically explored by varying the atomic concentration of each element between 5% and 35%. The temperature conditions ranged from 100 K to 1200 K in increments of 100 K. For each combination of composition and temperature, a uniaxial tensile test was conducted to measure the

UTS. The simulations were performed under periodic boundary conditions using the NPT ensemble, which ensures constant pressure and temperature during deformation. Atomic models were created using random substitution to achieve the desired alloy compositions. The simulation workflow followed the methodology outlined by Achmad et al. [8], integrating MD with thermodynamic and statistical analysis to evaluate mechanical properties. Each simulation generated stress–strain data, from which UTS values were derived. In total, 1812 unique simulations were conducted, resulting in a comprehensive dataset that captures the relationship between composition, temperature, and mechanical response. This dataset served as the foundation for subsequent machine learning analysis.

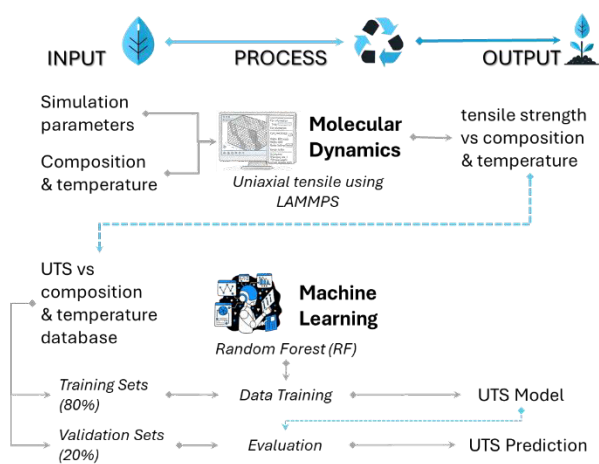


Fig. 2. Simplified workflow showing the integration of MD simulations and Random Forest ML to predict UTS from composition and temperature in FeNiCrCoAl HEAs.

2.2 Random Forest Machine Learning Method

The RF algorithm was chosen for its robustness, interpretability, and outstanding performance in regression tasks that involve complex, nonlinear relationships. The RF model was implemented in Google Colaboratory using the Scikit-learn library. The dataset was divided into 80% for training and 20% for testing to ensure a reliable evaluation of the model. To optimize prediction accuracy, hyperparameters such as the number of decision trees ($n_{estimators}$), maximum depth, and minimum samples per leaf were adjusted. The model was trained to learn the relationship between elemental composition, temperature, and UTS. It was then validated using standard metrics, including R^2 (coefficient of determination) and RMSE (root mean square error). To understand the influence of each input variable, a feature importance analysis was conducted. Additionally, Spearman's rank correlation was employed to assess the monotonic relationships between the features and the target properties. This methodology is consistent with our previous work, which demonstrated the effectiveness of the RF algorithm in predicting stacking fault energy and mechanical behavior in HEAs [8].

3 Results and Discussions

3.1 Molecular Dynamics Results

The mechanical performance of FeNiCrCoAl HEAs is profoundly influenced by temperature, a relationship clearly illustrated in Fig. 3. As temperatures rise, UTS experiences a consistent decline across all tested compositions. This intriguing phenomenon is primarily a result of thermally activated dislocation recovery. With increasing temperatures, atomic vibrations intensify, which weakens interatomic bonds and lowers the energy barriers for atomic rearrangement, thereby facilitating plastic deformation more readily. This process of thermal softening reduces the stress necessary for dislocation movement, prompting a transformation in the material's response from elastic to plastic and ultimately diminishing its tensile strength. Such behavior aligns seamlessly with previous molecular dynamics studies of CoCrCuFeNi HEAs, which similarly reveal reductions in both elastic modulus and UTS as temperatures escalate [10]. Furthermore, simulations involving FeNiCrMn HEAs highlight that heightened thermal vibrations weaken atomic bonding and diminish the critical resolved shear stress required for dislocation nucleation, creating more slip pathways for deformation [11]. The cumulative thermal energy not only accelerates dislocation annihilation but also results in a reduced overall dislocation density, undermining the material's capacity for work hardening. At exceptionally high temperatures, diffusion-controlled plasticity mechanisms, like creep, emerge as dominant forces, further compromising the tensile strength of these remarkable alloys [12].

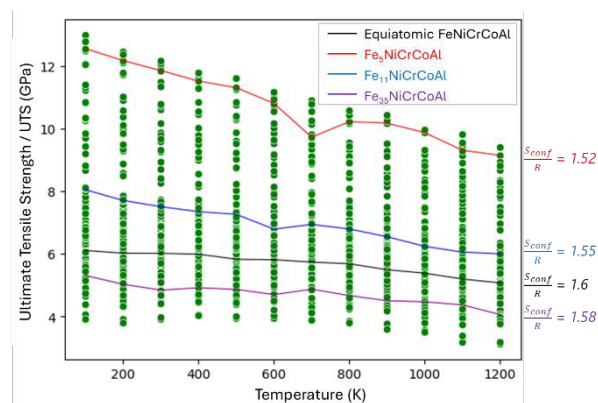


Fig. 3. Variation of Ultimate Tensile Strength (UTS) with temperature for different FeNiCrCoAl alloy compositions, showing the influence of configurational entropy (S_{conf}/R).

Fig. 3 vividly illustrates the relationship between UTS and temperature for a range of FeNiCrCoAl compositions, showcasing both equiatomic and non-equiatomic variants. Remarkably, the equiatomic alloy exhibits a modest decrease in UTS (approximately 6 GPa) across all temperatures, reflecting a commendable level of thermal stability. However, what truly captivates attention is the performance of certain non-equiatomic compositions, such as Fe₃NiCrCoAl ($S_{conf}/R = 1.52$), which possess lower configurational entropy than the equiatomic variant yet achieve nearly double the UTS across the entire temperature spectrum. This intriguing trend, however, is not universally

applicable. The composition $\text{Fe}_{35}\text{NiCrCoAl}$, with similarly low entropy, surprises with its notably lower UTS, illustrating that configurational entropy alone cannot solely account for mechanical performance. A complex interplay of elemental interactions, phase stability, and atomic-scale distortions governs the true mechanics at play. To enrich this analysis, Fig. 4 charts UTS against configurational entropy (S_{conf}/R), revealing an intriguing correlation: higher entropy values generally lead to lower tensile strength. While the entropy differences in this study are relatively modest (ranging from 1.52 to 1.60 R), they still yield significant variations in mechanical behavior. These findings highlight the need for precise compositional tuning, where both entropy and elemental interactions are key to optimizing HEA strength across temperatures.

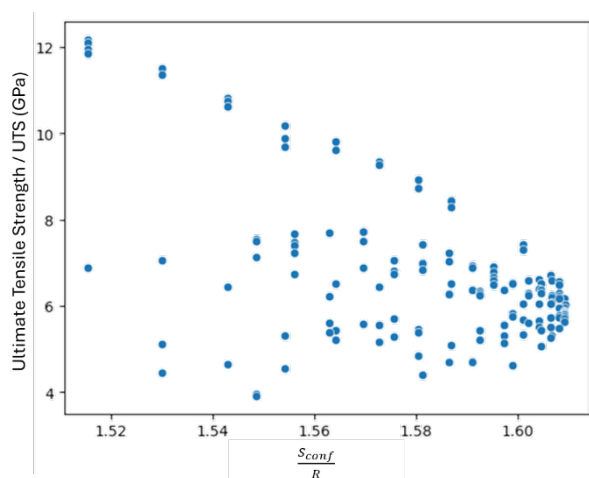


Fig. 4. Scatter plot showing the inverse relationship between UTS and configurational entropy (S_{conf}/R).

The variation in Al content reveals a captivating non-linear relationship with UTS, as depicted in Fig. 5. Initially, as Al concentration rises, UTS experiences a decline, reaching its lowest values around 15 - 20 atomic percent. Remarkably, beyond this threshold, UTS begins to ascend once more. This intriguing trend is illustrated by the red dashed line alongside a cluster of notable data points near 20 at.% Al. Here, compositions with Co, Cr, or Fe below 9 at.% achieve impressively higher UTS. This suggests that targeted reductions in these elements, paired with strategic adjustments in Al concentration, can significantly amplify mechanical performance. This striking behavior can be traced back to Al's low valence electron concentration (VEC) and its substantial atomic radius, both of which foster the stabilization of the body-centered cubic (BCC) phase and amplify lattice distortion [13]. While the emergence of the BCC structure bolsters strength, it simultaneously introduces brittleness and diminishes ductility, thus posing challenges to the alloy's performance under tensile stress [14]. Furthermore, Al plays a pivotal role in solid solution strengthening due to its size mismatch with other matrix elements, enhancing resistance to dislocation motion and elevating the overall robustness of the alloy.

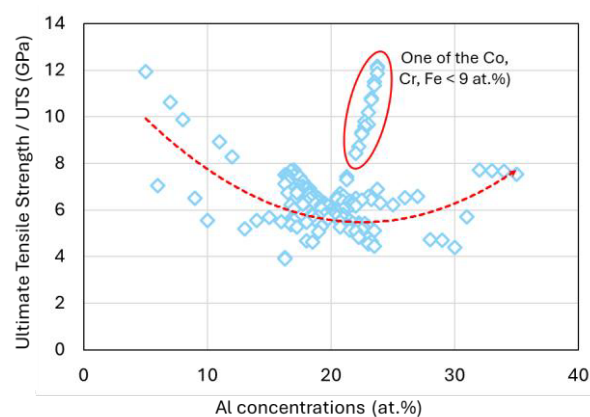


Fig. 5. Scatter plot showing the relationship between Al concentration and UTS in FeNiCrCoAl HEAs, with a red dashed trend line and highlighted region indicating enhanced UTS.

Fig. 6 presents another series of scatter plots that vividly illustrate the effects of atomic concentrations of Fe, Ni, Co, and Cr on UTS. Each plot also features a striking red dashed trend line and highlights specific compositional clusters where one or more elements hover around approximately 9 at.%, showcasing remarkably higher UTS. Echoing the behavior of Al, the data reveal a fascinating non-linear relationship between UTS and elemental concentration. Remarkably, Fe, Co, and Cr exert a substantial influence on tensile strength. At the same time, the impact of Ni concentration appears relatively subdued, as indicated by the minimal variation in UTS across the tested range. These insights highlight the critical importance of meticulous compositional tuning, particularly of Al, Fe, Co, and Cr, to unlock and optimize the mechanical performance of HEAs.

3.2 Random Forest Machine Learning Results

Fig. 7 highlights the predictive capability of the RF model in estimating the UTS of HEAs. Fig. 7(a) presents a scatter plot comparing predicted and actual values, where the data points closely align with the red diagonal line, indicating a strong correlation. The model achieves an R^2 value of 0.975, with a low Mean Squared Error (MSE = 0.06) and Root Mean Square Error (RMSE = 0.22), confirming its high accuracy. Fig. 2(b) further supports this by showing histograms of UTS distributions for actual (red) and predicted (blue) values, which exhibit similar patterns, demonstrating the model's ability to replicate the statistical behavior of the target property. The RF model operates by constructing an ensemble of decision trees during training and averaging their outputs to improve predictive performance. This approach enhances generalization and reduces variance, making RF particularly effective for modeling complex, nonlinear relationships among alloy composition, processing temperature, and mechanical behavior. In the context of HEAs, RF captures intricate interactions among compositional elements and processing parameters, while remaining resilient to overfitting and noise. Its ability to handle high-dimensional data and uncover hidden patterns makes RF a robust and reliable tool for forecasting

mechanical properties in advanced alloy systems, as also emphasized by Zhao et al. in their comprehensive

review of machine learning applications in HEA design [15].

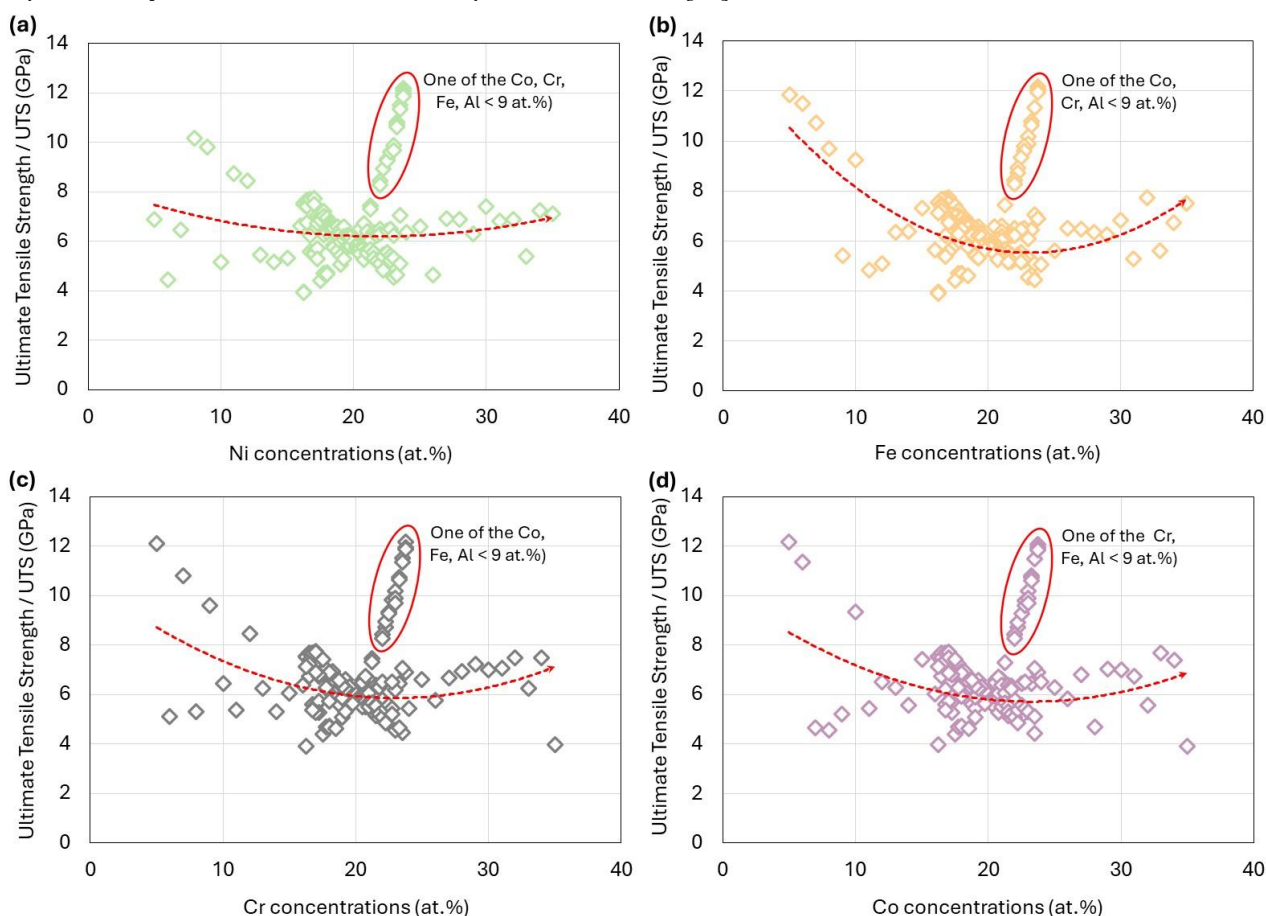


Fig. 6. Scatter plots showing the relationship between Ni, Fe, Cr, and Co concentrations and UTS in HEAs.

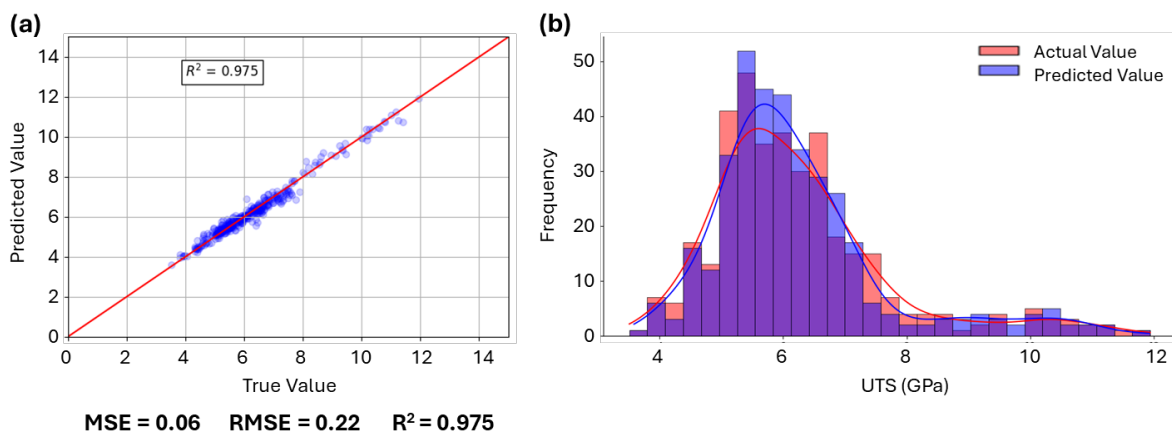


Fig. 7. Random Forest model performance in predicting UTS of HEAs: (a) scatter plot showing high correlation between predicted and actual values; (b) histogram comparing distributions of actual and predicted UTS values.

3.3 Design Guidelines for FeNiCrCoAl HEAs

Predictions of mechanical properties derived from MD simulations often do not align with actual values observed in HEAs. Instead, these simulations primarily serve to illustrate the influence of various parameters, rather than to provide definitive outcomes [8]. In this study, we delve into the compositional correlations within FeNiCrCoAl HEAs. Fig. 5 and Fig. 6 reveal U-shaped trends in UTS across varying atomic percentages

of Al, Ni, Fe, Cr, and Co, with high-strength outliers at specific ranges. Notably, Al and Cr exhibit significant variation in UTS at low concentrations, prompting an analysis of the top 10% high-UTS compositions across different temperatures. Although these low concentrations reduce configurational entropy, the data show that lower entropy does not always correlate with higher UTS, as illustrated in Fig. 3, where Fe at 11 at.% yields lower UTS than the equiatomic HEA with the highest entropy.

To investigate the influence of compositional and thermal parameters on mechanical properties in HEAs, we applied machine learning techniques, including Spearman's rank correlation and feature importance analysis. Spearman's rank correlation, shown in Fig. 8, identifies monotonic relationships—whether linear or nonlinear—between input features (Fe, Ni, Cr, Co, Al, and temperature) and mechanical outputs such as UTS. This method is particularly suitable for materials science datasets, where relationships between variables may not follow strict linear patterns. The analysis reveals that temperature has the strongest negative correlation (-0.32), followed by Al (-0.09), indicating their significant influence on mechanical behavior. Other elements show weaker correlations: Fe (0.01), Ni (0.03), Cr (-0.01), and Co (0.03). These insights help prioritize variables for further modeling and optimization, especially in complex alloy systems where nonlinear dependencies are common.

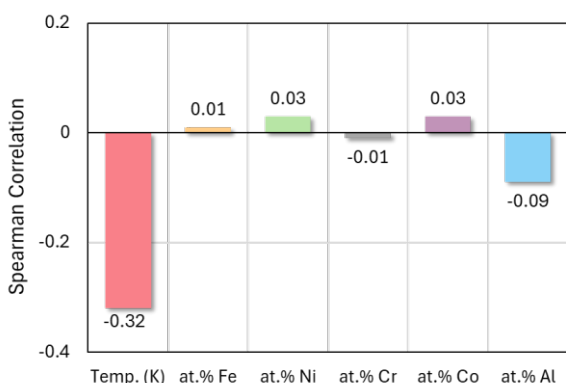


Fig. 8. Spearman's rank correlation coefficients indicating monotonic relationships between elemental composition, temperature, and UTS in the HEA system.

While Spearman's rank correlation identifies monotonic relationships—whether linear or nonlinear—between variables, feature importance quantifies the extent to which each feature contributes to reducing prediction error in a trained model, taking into account interactions and combined effects. As shown in Fig. 9, the feature importance distribution highlights the relative impact of elemental composition on mechanical properties, with Ni showing the highest importance (0.27), followed by Fe (0.20), Co (0.19), Al (0.17), and Cr (0.16). These results suggest that Ni plays a dominant role in influencing the target properties, particularly UTS. Interestingly, while Spearman's correlation identified temperature and Al as having strong monotonic relationships with mechanical properties, feature importance reveals that Ni and Fe are more influential in predictive modeling. This complementary use of both methods provides a more comprehensive understanding of the complex, nonlinear interactions among alloying elements and their effects on mechanical performance.

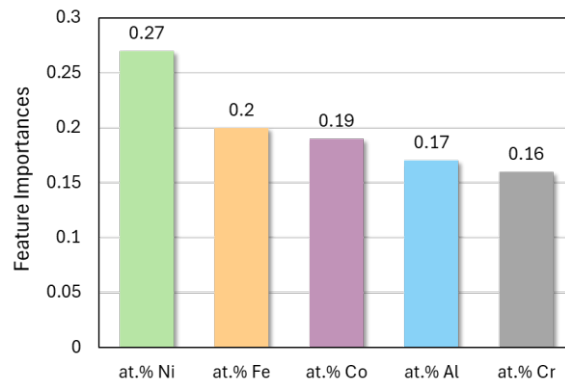


Fig. 9. Feature importances of elemental atomic percentages (Ni, Fe, Co, Al, Cr) in predicting mechanical properties of FeNiCrCoAl HEAs.

To strategically unlock the potential of FeNiCrCoAl HEAs for enhanced mechanical properties, we turned to the power of machine learning. This innovative approach allowed us to pinpoint optimal elemental compositions that significantly elevate performance. Our feature-based modeling revealed a fascinating insight: adjusting Cr to levels between 5–9 at.% and Al to 5–8 at.% can dramatically boost tensile strength. Moreover, maintaining elevated levels of Ni is crucial, as it plays a vital role in stabilizing the FCC phase. As illustrated in Fig. 10, our model has predicted two optimized compositions that achieve impressive UTS values of 12.17 GPa and 12.09 GPa at 25°C. Both formulations contain Co, Ni, and Fe at 23.5 at.%, while the levels of Al and Cr are cleverly balanced—one composition features low Al (5 at.%) and high Cr (23.5 at.%), while the other showcases high Al (23.5 at.%) and low Cr (5 at.%). This compelling comparison not only underscores the sensitivity of UTS to precise elemental adjustments but also highlights the transformative power of machine learning in guiding thoughtful and cost-efficient alloy design.

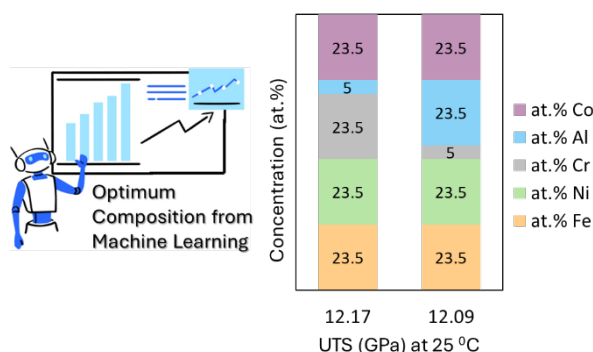


Fig. 10. Optimum compositions predicted by machine learning based on varying concentrations of Co, Al, Cr, Ni, and Fe.

4 Conclusions

1. Temperature and elemental composition significantly influence the UTS of FeNiCrCoAl HEAs. Temperature acts as the dominant softening factor, consistently reducing tensile strength across all compositions. Ni emerges as a key contributor to

strength, enabling targeted reduction of Co, Cr, and Al. The performance of certain non-equiatomic compositions, such as FeNiCrCoAl₅ and FeNiCr₅CoAl, which possess lower configurational entropy than the equiatomic variant, achieves nearly double the UTS across the entire temperature spectrum. The optimized alloy retained over 90% of its strength throughout the tested temperature range, demonstrating excellent thermal stability and mechanical resilience.

2. RF algorithm demonstrated high predictive accuracy, with an R² value of 0.975 and an RMSE of 0.22, effectively capturing the nonlinear relationships between composition, temperature, and UTS. Feature importance analysis identified Ni and Fe as the dominant predictors, while Spearman's rank correlation revealed temperature and Al as significant monotonic influencers.
3. Optimal UTS performance was achieved by tuning Cr and Al concentrations to 5–9 at.% and 5–8 at.%, respectively, while maintaining Ni at ≥20 at.% to stabilize the FCC phase. These findings provide a robust, data-driven guideline for designing high-performance HEAs with reduced reliance on critical elements and improved mechanical resilience.

This work was supported by the Research, Community Service, and Innovation (PPMI) Program ITB 2025 and the Research and Innovation Program for Advanced Indonesia (RIIM) 2023 BRIN.

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