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Investigation of the Impact of Alloying Elements on the Mechanical Properties of Superalloys Using Explainable Artificial Intelligence

Berkay Emin [*,1], **Yusuf Uzunoğlu** [α,2] **and Yusuf Alaca** [β,3]

[*]Electronics and Automation, Osmancik Omer Derindere Vocational College, Hitit University, Çorum, Türkiye, [α]Materials Science and Engineering, Erciyes University, 38039 Kayseri, Türkiye, [β]Computer Engineering, Hitit University, 19030 Çorum, Türkiye.

ABSTRACT This study investigates the impact of alloying elements on the mechanical properties of Ni-Cr-Fe-based superalloys using a computational materials science approach. Fifty different compositions of superalloys, commonly known as Inconel and Incoloy, were modeled using the JMatPro software. The mechanical properties, including 0.2% proof stress (MPa), fracture stress (MPa), and Young's modulus (GPa), were simulated across a temperature range from 540 °C to 920 °C at 20 °C intervals for each alloy. The simulation generated a comprehensive dataset comprising 1000 rows. This dataset was then utilized to train an explainable artificial intelligence (XAI) model, leveraging advanced techniques such as SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations), and Partial Dependence Plots (PDP). The dataset was analyzed using an XAI-based regression model employing the XGBoost algorithm. The interpretability graphs were analyzed to evaluate the individual contributions of each alloying element to the mechanical properties over the entire temperature range. The findings provide detailed insights into the positive or negative effects of alloying elements, enabling a better understanding of their role in optimizing superalloy performance under various thermal conditions. This work highlights the potential of integrating computational materials modeling and explainable AI to advance the design and development of high-performance materials.

KEYWORDS
Explainable artificial intelligence
Computational materials
Superalloys
mechanical properties

INTRODUCTION

Nickel-based superalloys have long been integral to industries requiring materials that sustain mechanical strength and resistance to oxidation at high temperatures, such as aerospace, power generation, and petrochemical applications (Hamdi and Abedi 2024). These alloys derive their exceptional properties from complex microstructures, primarily composed of austenitic γ-matrix and strengthening γ' or γ'' phases (Zhang *et al.* 2023). Elements like chromium, molybdenum, and aluminum are strategically added to enhance specific attributes, including oxidation resistance, creep strength, and precipitation hardening. However, the intricate interplay of these alloying elements under varying operational conditions remains a subject of extensive investigation (Monzamodeth *et al.* 2021).

Recent advancements in computational tools, such as JMatPro, have enabled high-throughput simulations of phase equilibria, mechanical properties, and thermal stability across a range of compositions and temperatures (Zhu *et al.* 2024). These simulations provide foundational insights for alloy design but often fail to elucidate the nuanced contributions of individual elements. Consequently, machine learning and explainable AI (XAI) approaches, such as SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations), have gained traction for interpreting the role of compositional variables in material properties (Zhang *et al.* 2024). These methods have proven effective in correlating microstructural features with performance metrics, such as proof stress and fracture toughness, particularly in alloys subjected to high-temperature deformation (Huang *et al.* 2024).

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[1]berkayemin@hitit.edu.tr (**Corresponding author**).
[2]4012640009@erciyes.edu.tr
[3]yusufalaca@hitit.edu.tr

The Ni-Cr-Fe alloy system, including widely used grades such as Inconel and Incoloy, exemplifies the importance of compositional control. Studies have shown that chromium improves oxidation resistance, while iron balances cost-effectiveness and thermal stability (Cheng *et al.* 2024). However, the presence of secondary phases, such as topologically close-packed (TCP) structures, can detrimentally impact mechanical properties, necessitating careful optimization of alloying elements and processing conditions (Zhang *et al.* 2023).

This study builds on the existing body of knowledge by integrating computational materials science and XAI methodologies to analyze the mechanical properties of Ni-Cr-Fe superalloys. By leveraging a dataset comprising simulations at incremental temperatures, it aims to quantify the contributions of each alloying element to properties like proof stress, fracture stress, and Young's modulus. The findings are expected to provide actionable insights for alloy design and performance optimization in high-temperature applications.

MATERIALS AND METHODS

This study employs a computational materials science approach combined with explainable artificial intelligence (XAI) to investigate the influence of alloying elements on the mechanical properties of Ni-Cr-Fe-based superalloys. Using JMatPro software, fifty different Ni-Cr-Fe alloy compositions, including Inconel and Incoloy, were modeled to simulate mechanical properties such as 0.2% Proof Stress (MPa), Fracture Stress (MPa), and Young's Modulus (GPa) over a temperature range of 540°C to 920°C at 20°C intervals. The simulations produced a dataset comprising 1000 entries, which served as input for an XAI-driven regression model utilizing the XGBoost algorithm. This model enabled the generation of SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations), and PDP (Partial Dependence Plots) to elucidate the contribution of individual alloying elements to the mechanical properties across the temperature range.

Figure 1 illustrates the proposed model workflow, detailing the integration of computational simulations, dataset generation, machine learning model training, and XAI-based interpretative analysis. This framework aims to provide comprehensive insights into how each alloying element influences mechanical performance, paving the way for optimized superalloy design tailored to high-temperature applications.

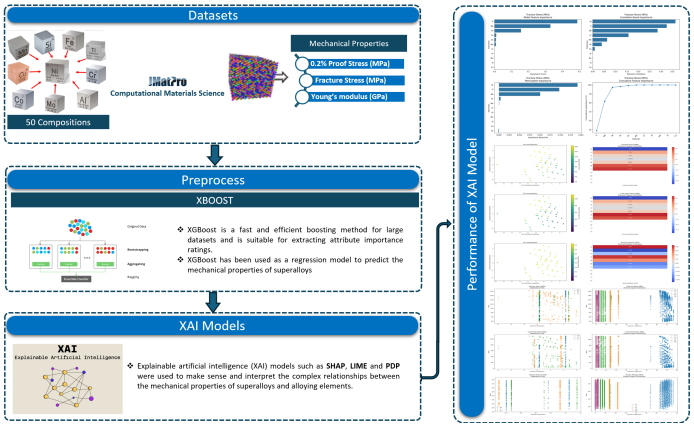

Figure 1 Proposed Model

Dataset Preparation

This study focuses on Ni-Cr-Fe-based superalloys, such as Inconel and Incoloy, widely used in industry due to their high mechanical performance and ability to undergo precipitation hardening through solution treatment and aging processes. These heat treatment procedures stabilize the microstructure and enhance the material's ability to maintain mechanical properties at elevated temperatures over prolonged periods. Precipitation hardening is a key process that significantly improves the strength of Inconel and Incoloy alloys at high temperatures (Zhang 2019).

The compositions modeled in JMatPro were based on key elements of Ni-Cr-Fe superalloys, including Ni, Cr, Fe, Co, Mo, Nb, and Ti. Elements such as Al, Mn, Si, and Cu, which enable precipitation hardening and aging treatments, were held constant at specific levels across all alloy combinations (ASM International 1991). The alloy compositions were designed to optimize their mechanical properties by simulating the solution treatment and aging parameters. The weight fractions of the primary elements were varied within the following ranges: 50–75% Ni, 14–21% Cr, 5–15% Fe, 0–2% Co, 0–3% Mo, 1–5% Nb, and 1–2.5% Ti. Additionally, the following weight fractions were kept constant in all compositions: 0.5% Al, 1% Mn, 0.5% Si, and 0.5% Cu. Phase Fraction Diagrams and TTT (Time-Temperature-Transformation) Diagrams were generated for each alloy composition. Table 1 outlines the range of alloying elements used to design 50 distinct alloy compositions. Each composition was evaluated across 20 different temperatures ranging from 540°C to 920°C, in increments of 20°C. The simulated mechanical properties - 0.2% Proof Stress (MPa), Fracture Stress (MPa), and Young's Modulus (GPa) - were recorded for each temperature. As a result, a comprehensive dataset consisting of 50 alloy compositions and their mechanical properties across 20 temperature points was developed, yielding a total of 1,000 data rows.

Table 1 Elemental Composition Ranges of Alloys in the Dataset (values represent wt%)

Ni (%)	Cr (%)	Fe (%)	Co (%)	Mo (%)	Nb (%)	Ti (%)	Al (%)	Mn (%)	Si (%)	Cu (%)
50–75	14–21	5–15	0 and 2	0 and 3	1 and 5	1 and 2.5	0.5	1	0.5	0.5

Table 2 illustrates an example of the dataset, showcasing two alloy compositions. The second alloy composition differs from the first by the addition of 1% Co, which is observed to enhance the mechanical property values. This dataset serves as the foundation for subsequent analysis, enabling the systematic investigation of how individual alloying elements influence the mechanical behavior of superalloys under various thermal conditions.

Heat Treatment Simulation and Microstructure Optimization The simulations for this study were performed using the JMatPro software, which is based on principles of computational materials science. The software was used to model 50 different compositions of Ni-based superalloys, with specific alloying elements added to nickel at varying proportions. For each composition, Phase Fraction Diagrams and TTT (Time-Temperature-Transformation) Diagrams were generated and analyzed to determine the optimal heat treatment temperature for forming the two precipitate phases, gamma prime (γ') and gamma double prime (γ''). These phases were selected as they contribute significantly to the mechanical

Table 2 The First Two Compositions (C1, C2) in the Dataset

Ni (%)	Cr (%)	Fe (%)	Co (%)	Mo (%)	Nb (%)	Ti (%)	Al (%)	Mn (%)	Si (%)	Cu (%)	Temperature (ºC)	0.2% Proof Stress (MPa)	Fracture Stress (MPa)	Young's Modulus (GPa)
67	22	5	0	0	1	2.5	0.5	1	0.5	0.5	920.0	89.27	332.99	137.5
67	22	5	0	0	1	2.5	0.5	1	0.5	0.5	900.0	165.08	551.78	139.74
67	22	5	0	0	1	2.5	0.5	1	0.5	0.5	880.0	218.35	729.71	141.92
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
67	22	5	0	0	1	2.5	0.5	1	0.5	0.5	580.0	768.34	1380.38	168.64
67	22	5	0	0	1	2.5	0.5	1	0.5	0.5	560.0	767.79	1392.7	170.14
67	22	5	0	0	1	2.5	0.5	1	0.5	0.5	540.0	767.28	1404.43	171.62
66	22	5	1	0	1	2.5	0.5	1	0.5	0.5	920.0	110.51	387.26	138.29
66	22	5	1	0	1	2.5	0.5	1	0.5	0.5	900.0	176.07	582.59	140.53
66	22	5	1	0	1	2.5	0.5	1	0.5	0.5	880.0	226.97	756.4	142.73
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
66	22	5	1	0	1	2.5	0.5	1	0.5	0.5	580.0	770.05	1382.07	169.35
66	22	5	1	0	1	2.5	0.5	1	0.5	0.5	560.0	769.51	1394.4	170.85
66	22	5	1	0	1	2.5	0.5	1	0.5	0.5	540.0	769.02	1406.14	172.34

properties of the alloys (Peachey *et al.* 2024). The resulting mechanical property values at the determined temperatures were incorporated into the dataset.

Each composition was simulated using heat treatment parameters tailored to produce gamma (γ), gamma prime (γ'), and gamma double prime (γ'') phases while excluding undesired phases such as delta, eta, laves, MC, M6C, and M3B2. These phases were disregarded due to their formation only during prolonged aging processes and their potential to negatively affect mechanical properties (Schulz *et al.* 2024). The simulations were performed under equilibrium conditions, ensuring that unwanted phases, which would typically appear under extremely slow cooling or extended durations in real-world applications, were excluded. This approach enabled the modeling of results that accurately reflect practical heat treatment processes. The grain size of the matrix phase (gamma)

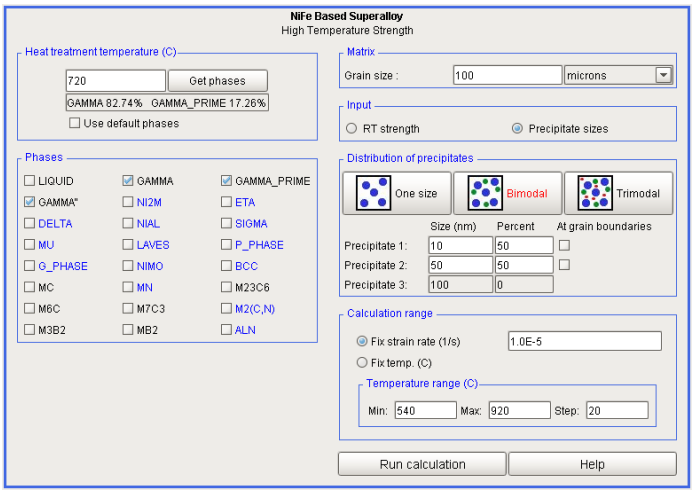

Figure 2 Input Parameters and Bimodal Distribution Settings for Ni-Based Superalloy Simulation in JMatPro

was set at 100 microns, while the precipitate sizes for gamma prime (γ') and gamma double prime (γ'') phases were defined as 10 nm and 50 nm, respectively. To simulate the microstructure effectively, the "Bimodal" distribution option was selected, as shown in Figure 2. The heat treatment parameters, including temperature and duration, were optimized for each composition to ensure the complete precipitation of gamma prime (γ') and gamma double prime (γ'') phases within the matrix (Gontcharov and Lowden 2024). The temperature range for these simulations was set between 540°C and 920°C, ensuring a comprehensive evaluation of the material's mechanical properties across relevant service conditions.

The results from these simulations provided critical insights into the microstructure and mechanical properties of the modeled alloys, serving as the foundation for further analysis and optimization.

Development of the Explainable Artificial Intelligence Model In this study, a powerful machine learning algorithm, the XGBoost regression model, is used and Explainable Artificial Intelligence (XAI) methods are integrated to ensure the explainability of the artificial intelligence model developed for the prediction of mechanical properties of Ni-Cr-Fe based superalloys.

XGBoost (Extreme Gradient Boosting) is a high-performance and scalable gradient boosting algorithm widely used in machine learning. Developed by Chen and Guestrin (2016), this method is particularly notable for its capacity to achieve effective results on large datasets and high-dimensional feature spaces. XGBoost is a decision tree-based model that gradually adds new trees at each iteration to reduce errors. This process aims to minimize overfitting while increasing the generalization capability of the model. Furthermore, XGBoost's regularization techniques keep the model's complexity under control, resulting in more robust and reliable predictions. Thanks to its parallel processing capabilities and optimized computational processes, XGBoost outperforms other gradient boosting algorithms in terms of both speed and accuracy. Thanks to these features, XGBoost has a wide range of applications in both academic research and industrial applications (Chen and Guestrin 2016).

To make the inner workings and decision-making processes of the model transparent, widely accepted XAI methods such as SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-Agnostic Explanations) and Partial Dependence Plots (PDP) were used.

SHAP is an advanced explainable artificial intelligence (XAI) method developed to interpret the predictions of machine learning models transparently and understandably. Using Shapley values based on game theory, SHAP distributes the contribution of each feature to model prediction fairly and consistently. This approach reveals the inner workings of complex and black box models, making the reasons for model decisions more understandable for users. SHAP, as defined by Lundberg and Lee (2017), can provide both local (for individual forecasts) and global (model-wide) explanations. One of the key advantages of SHAP is that it is compatible with different types of models and can work model independently, making it ideal for a wide range of applications. Furthermore, the descriptions obtained with SHAP provide reliability and transparency for model users, which increases model acceptance, especially in high-risk areas (Lundberg and Lee 2017).

LIME is an explainable artificial intelligence (XAI) method developed to make the predictions of complex machine learning models locally understandable and interpretable. This method, described by Ribeiro, Singh, and Guestrin (2016), creates a simple and local model to explain a particular prediction of any model. LIME generates new data around a specific data point decided by the target model and trains a simple model (e.g., linear regression) on this data, trying to understand the behavior of the original model on this data point. In this way, it provides a visual and quantitative representation of how complex and black box models are affected by which inputs for certain predictions. LIME's model-agnostic nature makes it compatible with different machine learning algorithms and offers a wide range of applications. These features make LIME a valuable tool for engineering-oriented problems such as the optimization of mechanical properties of superalloys Ribeiro *et al.* (2016).

Partial Dependence Plots (PDPs) are an analysis method used in machine learning models to visualize the effect of one or more features on the model output. PDPs show, on average, how the model's predictions change if the value of the examined feature changes while all other features are held constant. This method is particularly important for understanding the general trends of complex and so-called black box models and for interpreting the effects of specific features on the model. The PDPs developed by Friedman (2001) allow us to better understand the effects of features on target variables such as mechanical properties by revealing how the model reacts to which features. This makes it possible to determine which elements and ranges are critical in optimizing the mechanical properties of superalloys (Friedman 2001).

RESULTS AND DISCUSSION

In this chapter, a comprehensive analysis of the effect of alloying elements on the mechanical properties of Ni-Cr-Fe based superalloys is presented by using descriptive artificial intelligence (XAI) methods. The study modeled the mechanical properties (tensile strength, proof stress, and modulus of elasticity) at temperatures between 540°C and 920°C for 50 different compositions and analyzed these data with XAI methods to highlight the effects of alloying elements.

In the study, data generated with JMatPro software were analyzed with an XAI-based regression model shaped using the XGBoost algorithm. The findings revealed the significant effects of elements such as Titanium (Ti), Niobium (Nb), and Nickel (Ni) on tensile strength and proof stress, while emphasizing the importance of Cobalt (Co) and Molybdenum (Mo) for the modulus of elasticity. The visibility obtained from the XAI analyses details numerically and graphically the positive and negative effects of each element on the mechanical properties, and a meaningful roadmap for alloy design is presented below. Figure 3 presents the results

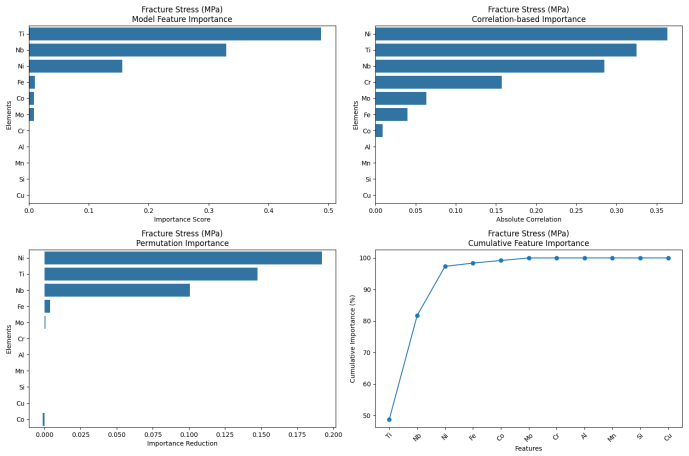

Figure 3 Importance of Alloying Elements on Fracture Stress (MPa)

of different analysis methods to explain the influence of alloying elements on Fracture Stress. The model feature importance plot shows the feature importance scores determined by the artificial intelligence model. In this analysis, Titanium (Ti) stands out as the element with the highest influence, while Niobium (Nb) and Nickel (Ni) rank second and third, respectively. Other elements such as Fe (Iron), Mo (Molybdenum), and Cr (Chromium) have lower levels of significance. This suggests that the effects on fracture strength are largely associated with Ti, Nb, and Ni.

The correlation-based importance graph evaluates the linear relationship between the fracture stress and each element based on absolute correlation values. According to this method, Nickel (Ni) has the highest correlation coefficient and shows a strong influence on fracture strength. Titanium (Ti) and Niobium (Nb) also exhibit high correlation values on fracture strength, while elements such as Cr and Mo have a lower effect. This analysis provides an important perspective to quantify the magnitude of direct and indirect effects on fracture strength.

Permutation importance plot is another analysis method that evaluates the contribution of each element to model performance. According to this method, Nickel (Ni) was identified as the most important element for model performance, followed by Titanium (Ti) and Niobium (Nb). The contributions of Fe, Mo, and Cr are relatively low. These results indicate that Ni, Ti, and Nb are the elements that improve the fracture stress prediction performance of the model the most.

Finally, the cumulative feature importance graph describes the cumulative impact of the features on the model. As can be seen in the graph, the combined contributions of Titanium (Ti), Niobium (Nb), Nickel (Ni), and Iron (Fe) together explain more than 90% of the model performance. The total contribution of the other elements is very limited. This indicates that the content ratios of these four elements should be optimized properly in the design of high-performance superalloys. Figure 4 contains the results evaluating the effects of alloying elements on 0.2% Proof Stress by different analysis methods.

The model feature importance plot shows the feature importance scores calculated by the artificial intelligence model. This analysis reveals that Titanium (Ti) and Niobium (Nb) have the highest impact on proof stress. After these two elements, Nickel

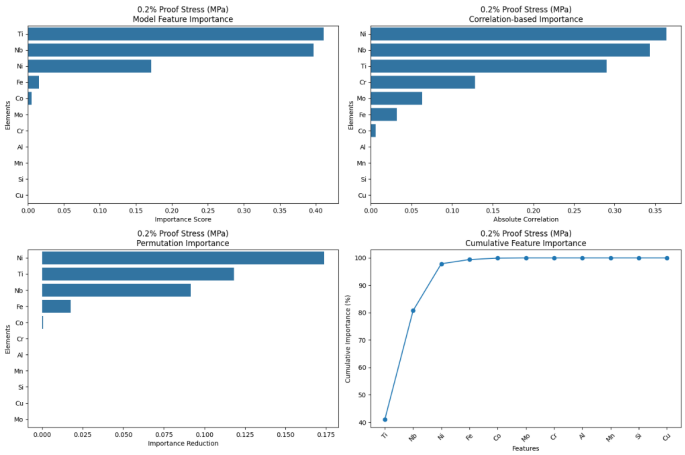

Figure 4 Importance of Alloying Elements 0.2% Proof Stress (MPa)

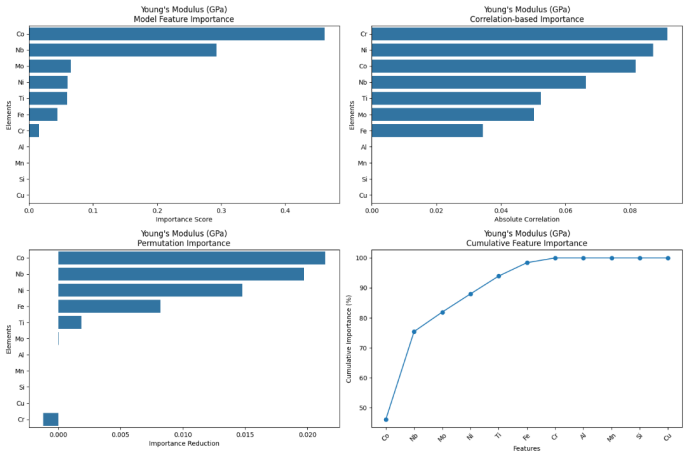

Figure 5 Importance of Alloying Elements on Young's Modulus (GPa)

(Ni) and Iron (Fe) contribute with lower importance levels. The effect of other elements (Co, Cr, Mo, Al, etc.) on model performance is very limited. These results emphasize that Ti and Nb are critical for 0.2% proof stress.

The correlation-based importance plot evaluates the linear relationship of each element with proof stress based on correlation. Here, Nickel (Ni) stands out as the element with the highest correlation coefficient. Niobium (Nb) and Titanium (Ti) rank second and third respectively, while other elements such as Cr and Mo show moderate correlation. This graph reveals that Ni has a significant influence on proof stress and that the contributions of Nb and Ti are also significant.

The permutation importance plot evaluates the contribution of the properties to the model performance in a commutativity-based approach. In this method, Nickel (Ni) is identified as the element with the highest impact on proof stress. Ti and Nb are ranked second and third in this order, with other elements such as Fe contributing less. Permutation-based analysis shows that Ni, Ti, and Nb play a key role in explaining model performance.

Finally, the cumulative feature importance plot shows how much the alloying elements explain the model performance in total. This graph shows that Titanium (Ti), Niobium (Nb), Nickel (Ni), and Iron (Fe) can explain more than 90% of the total model performance. The cumulative contribution of the other elements is very low. This suggests that the content ratios of these four elements should be prioritized to optimize the 0.2% proof stress.

Figure 5 presents the findings of various analytical methods that examine the effects of alloying elements on Young's Modulus determination. The model features an importance plot that reveals the importance ranking of the elements that contribute to the predictive power of the model. The results show that Cobalt (Co) in particular has a strong influence on Young's Modulus, followed by Niobium (Nb), Molybdenum (Mo), and Nickel (Ni). This kind of significance analysis makes it clear which elements need to be considered more to improve the mechanical properties.

Another method of analysis, the correlation-based importance plot, investigates whether each element has a linear relationship with Young's Modulus. This approach shows that Chromium (Cr) has the highest linear relationship, with elements such as Nickel (Ni) and Cobalt (Co) making significant contributions to this relationship. However, it should be noted that in this method, the influence of elements on mechanical properties may not be limited to correlation alone. This suggests that Cr may have a more significant effect than expected under some conditions.

The permutation importance plot evaluates the weight of elements in model performance from a different perspective. Here, Cobalt (Co) again emerges as the leading element, followed by Niobium (Nb) and Nickel (Ni). This type of analysis highlights the need to integrate these elements more intensively into the design process to improve Young's Modulus.

Finally, the cumulative feature importance plot provides an overall picture of how much the elements together explain the model performance. It can be seen that the contributions of Co, Nb, and Mo explain a large part of the model performance, while the other elements make only marginal contributions. This indicates the importance of optimizing the doping ratios in designs for enhancing mechanical properties. Figure 6 comprehensively

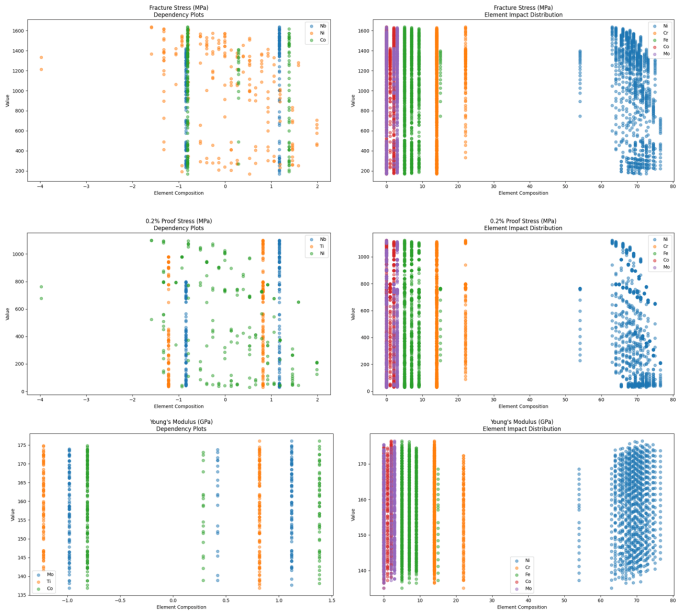

Figure 6 Dependence and Effect Distribution of Alloying Elements on Mechanical Properties

evaluates the effects of alloying elements on mechanical properties, both in terms of dependence and influence distribution. Firstly, the

analysis on Fracture Stress reveals that elements such as Niobium (Nb), Nickel (Ni), and Cobalt (Co) play a critical role in this mechanical property. In particular, a steady increase in fracture stress was observed with increasing Nb content. This trend emphasizes that Nb is a key element in terms of fracture strength. Similarly, Ni and Co also have significant effects on fracture stress, but these effects are concentrated in certain content ranges. The elemental influence distribution plots clearly show that the influence of Ni on the fracture stress is more dominant than that of the other elements and affects a wider range of contents.

Analysis of 0.2% Proof Stress shows that increasing the content of Nb and Ni significantly increases this property. These two elements are critical for optimizing proof stress. It was also observed that other elements such as Titanium (Ti) also have a positive contribution to proof stress, but the effect is not as dominant as Nb and Ni. The effect distribution plots emphasize the effects of Ni and Chromium (Cr) on this mechanical property, while Ni's strong influence on proof stress is once again confirmed. These analyses suggest that the Ni and Nb content ratios should be carefully controlled to improve the proof stress of superalloys.

Evaluations on Young's Modulus show that Molybdenum (Mo), Niobium (Nb), and Titanium (Ti) have positive effects on this mechanical property. In particular, it is noteworthy that an increase in the content ratio of Mo leads to a steady and significant improvement in the modulus of elasticity. This effect of Mo suggests that it plays a key role in improving elasticity. Nb and Ti also made significant contributions to Young's Modulus at certain content ranges and improved the mechanical performance of the superalloys. The effect distribution plots present the effects of Co and Nb on elasticity in a broad perspective, emphasizing the importance of these elements. Figure 7 presents a combination of Principal Component Analysis (PCA) and heat maps evaluating the correlation of elements with mechanical properties in superalloys. The graphs address three key mechanical properties, namely Fracture Stress, 0.2% Proof Stress, and Young's Modulus. The PCA visualizations present how the data is distributed in high-dimensional space reduced to two principal component axes, while the heat maps show the linear correlation of each element with these mechanical properties.

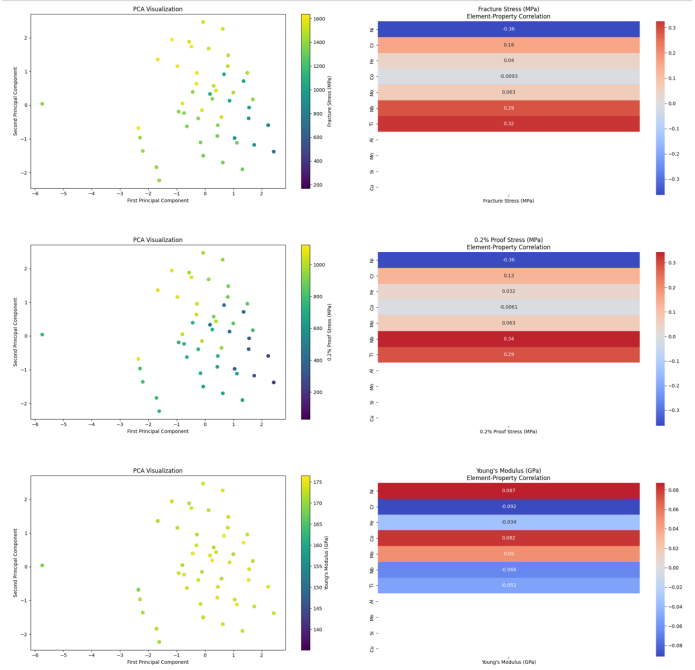

Figure 7 PCA Visualization and Element-Mechanical Property Correlations

The PCA visualization for Fracture Stress reveals that the data follow a specific distribution pattern and how this mechanical property can be correlated with different element compositions. The correlation heatmap shows that Niobium (Nb) has a negative correlation (-0.36), while Nickel (Ni) has a positive correlation (0.32). This indicates that Nb tends to decrease the fracture stress, while Ni has an increasing effect. The effects of Cobalt (Co) and other elements are relatively less pronounced.

The PCA analysis for 0.2% Proof Stress shows a similar distribution pattern, but the correlation map highlights the differences in the elements affecting this property. Nb again has a negative correlation (-0.36), whereas Ni (0.34) and Chromium (Cr, 0.29) stand out with positive correlations. This finding indicates that Nb has a decreasing effect on proof stress, while Ni and Cr improve this property.

The PCA visualization for Young's Modulus shows a more homogeneous distribution. The correlation map highlights that Molybdenum (Mo) has a significant positive effect (0.08) on the modulus of elasticity. In contrast, the effects of Nb and other elements on the modulus of elasticity are more limited. This confirms that Mo is one of the most critical elements for increasing elasticity.

According to the results given in Table 3, the developed model predicts the 0.2% Proof Stress and Fracture Stress properties of superalloys with reasonable accuracy (R^2 = 0.21 and 0.18). Low RMSE and MAE values indicate the reliability of the predictions. Although the performance of Young's Modulus could be improved, overall the model is considered a valuable tool in understanding the mechanical properties of superalloys. Figure 8 shows that the model has achieved significant success in understanding the relationships between mechanical properties and alloying elements. In particular, the results of the element complexity analysis revealed that Titanium (Ti) and Niobium (Nb) play a critical role in Fracture Stress and 0.2% Proof Stress, while Cobalt (Co) and Molybdenum (Mo) play a prominent role in Young's Modulus. This shows that

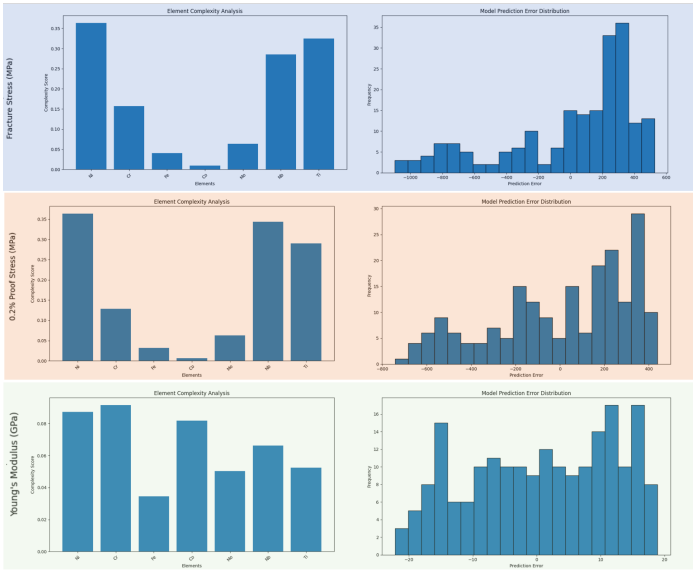

Figure 8 Element Complexity Analysis and Model Error Distribution

Table 3 Model Performance Metrics for Predicting Mechanical Properties

Property	Mean Squared Error	Root Mean Squared Error	R-squared	Mean Absolute Error	Mean Absolute Percentage Error	Cross-Validation R2 Mean	Cross-Validation R2 Std
0.2% Proof Stress (MPa)	95077.41	308.35	0.21	266.15	1.79	0.18	0.09
Fracture Stress (MPa)	171941.42	414.66	0.18	338.22	0.65	0.18	0.05
Young's Modulus (GPa)	125.25	11.19	-0.12	9.73	0.06	0.01	0.01

the model can accurately determine which elements make a greater contribution to optimizing mechanical properties. Moreover, when the distribution of prediction errors is analyzed, Young's Modulus predictions are within a narrow error range, indicating that the model works with high consistency for this property. The fact that the prediction errors for Fracture Stress and 0.2% Proof Stress are generally concentrated in a reasonable range also supports the overall accuracy of the model. These findings show that the model can provide reliable predictions for the design of superalloys in high-temperature applications and can be used as an effective tool for optimizing the effects of alloying elements. The results presented in Figure 9 show that the model can predict the Fracture Stress (MPa) and 0.2% Proof Stress (MPa) with significant accuracy. In particular, the relationship between predicted values and actual values for these two mechanical properties indicates that the model performs reliably in these areas. The positive trends observed in the R^2 distribution support the model's ability to consistently explain these properties and provide accurate predictions. This indicates that the model has effectively learned the interactions between alloying elements and mechanical properties. These results demonstrate that the model is a reliable tool for predicting critical mechanical properties such as Fracture Stress and 0.2% Proof Stress, which can provide useful insights in alloy design.

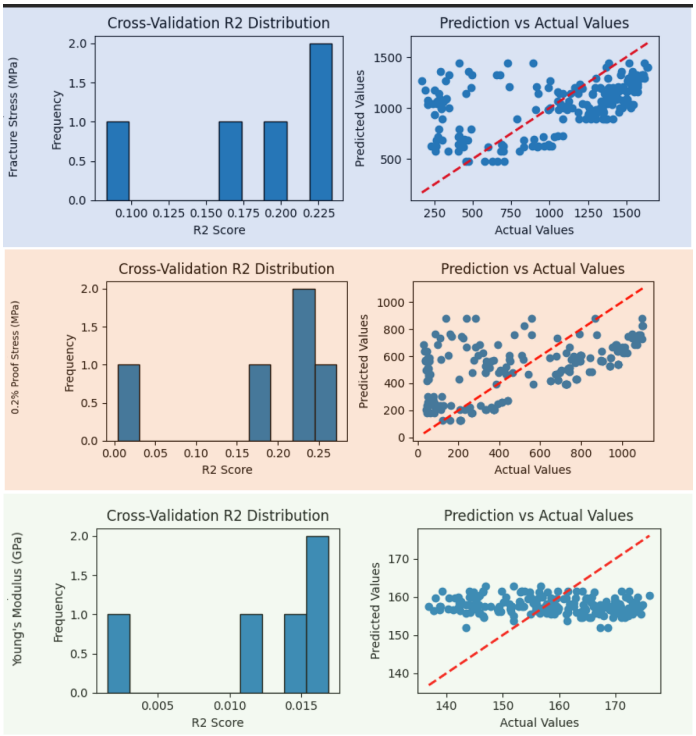

Figure 9 Cross Validation R^2 Distribution and Prediction vs Actual Value

CONCLUSION

This study comprehensively investigated the mechanical properties of Ni-Cr-Fe based superalloys under different alloying elements and temperature ranges through computational materials science approaches and explainable artificial intelligence (XAI) methods. The large data set obtained as a result of simulations performed between 540°C and 920°C in 20°C increments was analyzed with the XGBoost-based regression model and interpreted in depth using XAI techniques such as SHAP, LIME and PDP. These methods revealed that critical mechanical properties such as 0.2% proof stress, fracture stress and Young's modulus are strongly influenced by Nb, Ti, Ni, Co and Mo content.

The findings show that the effects of certain alloying elements on mechanical properties at different temperature conditions can vary both quantitatively and qualitatively. For example, elements such as Nb and Ni were found to play more prominent roles on fracture stress and proof stress with increasing temperature, while elements such as Mo and Co showed remarkable contributions in terms of Young's modulus at elevated temperatures. This shows that mechanical properties are not only dependent on chemical composition but also on thermal conditions, which necessitates the optimization of alloy designs to provide stabilized and durable performance at elevated temperatures.

The obtained data and analyses emphasize that elemental contents and operating temperatures should be strategically determined in the design of high-performance superalloys. In particular, the use of elements such as Nb, Ni, Ti, Co and Mo in the right proportions will provide superior performance in terms of fracture stress and proof stress at high temperatures, while keeping elastic properties under control. In this context, the present findings provide important guidance for future research and industrial applications.

Availability of data and material

Not applicable.

Conflicts of interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

Ethical standard

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

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