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High-Accuracy Prediction of Mechanical Properties of Ni-Cr-Fe Alloys Using Machine Learning

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ABSTRACT Artificial intelligence-driven prediction models have emerged as powerful tools for estimating material properties with high accuracy, yet the preparation of training datasets often demands labor-intensive and time-consuming experimental procedures. Leveraging the Computational Materials Science (CMS) approach, this study utilizes phase transformation calculations and thermodynamic data to simulate the mechanical properties of Ni-Cr-Fe alloys. Using JMatPro software, mechanical properties (0.2% Proof Stress, Fracture Stress, and Young's Modulus) of 50 Ni-Cr-Fe alloy compositions were simulated across a temperature range of 540–920 ℃, generating a dataset of 1000 rows. This dataset was used to train an Artificial Neural Network (ANN) model, with 80% allocated for training and 20% for validation and testing. The trained AI model demonstrated robust predictive capabilities, achieving a 96.61% accuracy rate in forecasting material compositions with the desired thermo-physical properties at specific temperatures. To validate the model's reliability, predicted alloy compositions were re-simulated under identical conditions in JMatPro, confirming the high fidelity of the model's predictions. The results underscore the efficacy of Computational Materials Science (CMS)-generated datasets as a scalable and reliable source for training AI models in materials science. This study highlights the potential of integrating Computational Materials Science (CMS) and Machine Learning approaches to accelerate material design and development processes, delivering significant improvements in prediction speed and accuracy.

KEYWORDS
Computational materials science
Machine learning
Artificial neural networks
Alloy design
Nickel alloys

INTRODUCTION

The development of predictive tools for estimating material properties has become increasingly important in the design and optimization of advanced alloys. Machine Learning (ML), as a data-driven approach, has shown remarkable potential in this domain by enabling the rapid prediction of mechanical, thermal, and thermodynamic properties. Recent studies highlight the effectiveness of Machine Learning models in understanding the complex interactions in multi-component systems such as Ni-Cr-Fe alloys, which are critical for high-performance applications due to their exceptional mechanical strength and corrosion resistance at elevated temperatures (Jain *et al.* 2023; Wang *et al.* 2021). These alloys are extensively used in aerospace, power generation, and chemical industries, where the optimization of their mechanical properties, such as yield strength, fracture toughness, and elasticity, is crucial (Mukhamedov *et al.* 2021).

Traditionally, experimental characterization of material properties has been labor-intensive, requiring extensive resources and time. The emergence of Computational Materials Science (CMS) has revolutionized this field by providing simulation-based insights into phase stability, stress-strain behavior, and thermodynamic properties. Tools like JMatPro have been instrumental in simulating the behavior of alloys under varied conditions, generating reliable datasets for machine learning applications (Filipoiu and Nemnes 2020; Liu *et al.* 2024). Leveraging these simulated datasets, Machine Learning models such as Artificial Neural Networks (ANNs) have demonstrated superior predictive accuracy, as seen in studies that model phase stability and hardness of high entropy alloys and other multi-component systems (Jeon *et al.* 2022; Chen *et al.* 2014).

In the context of Ni-Cr-Fe alloys, Machine Learning models have been utilized to explore the effects of compositional variations and temperature on mechanical properties. Studies employing physics-informed ML algorithms have successfully predicted thermodynamic and kinetic behaviors of chromium atoms in Fe-Ni-Cr systems, enhancing the understanding of stress-strain responses (Wang *et al.* 2021). Additionally, Machine Learning (ML)-driven methods have enabled the optimization of alloy compositions to achieve desired ductility, hardness, and elastic modulus (Jeon *et al.* 2022). Such approaches not only reduce dependency on experimental trials but also provide a pathway for exploring large compositional spaces effectively.

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This study aims to build upon these advancements by integrating Computational Materials Science (CMS) simulations and Machine Learning to predict the mechanical properties of Ni-Cr-Fe alloys. Using a dataset of 1000 rows simulated with JMatPro, an ANN model is trained to predict 0.2% proof stress, fracture stress, and Young's modulus across a temperature range of 540–920°C. The results indicate an accuracy exceeding 96.61%, demonstrating the robustness of this methodology. This work underscores the potential of combining simulation and Machine Learning to enhance alloy design, providing significant improvements in speed and precision compared to traditional methods.

MATERIALS AND METHODS

This study employs a Computational Materials Science (CMS)-based approach, leveraging the JMatPro software to simulate the mechanical properties of Ni-Cr-Fe-based nickel alloys. JMatPro, recognized for its ability to compute phase diagrams and thermodynamic properties, was utilized to generate a dataset comprising 1000 rows. These entries encompassed the mechanical properties of 50 distinct compositions, including elements such as Ni, Cr, Fe, Co, Mo, Nb, Ti, Al, Mn, Si, and Cu. The primary mechanical properties under investigation were 0.2% Proof Stress, Fracture Stress, and Young's Modulus, simulated across a temperature range of 540–920°C. The dataset was split into training (80%) and validation/testing (20%) subsets for model development and evaluation.

A Machine Learning (ML) model, specifically an Artificial Neural Network (ANN), was constructed to predict the mechanical properties of these alloys based on the CMS-generated dataset. As depicted in Figure 1, the model operates on a normalized dataset, where all input values were scaled between 0 and 1 using the Min-Max Normalization method. This preprocessing step ensures that the data are uniformly represented, facilitating effective learning by the ANN. To enhance dataset quality, missing values were addressed through multiple linear regression, ensuring the integrity and completeness of the input data. Additionally, all physical properties were converted into international SI units for consistency and further normalized before feeding into the model.

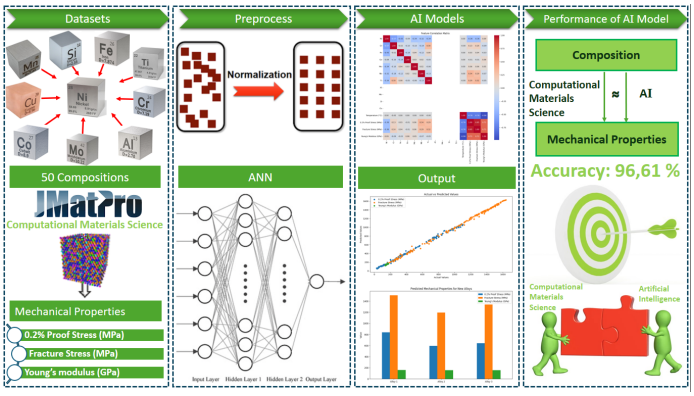

Figure 1 Flowchart of the proposed model for predicting the mechanical properties of Ni-Cr-Fe based nickel alloys

The proposed model (Figure 1) integrates the normalized data into a tensor structure, enabling efficient processing by the ANN architecture. The ANN was designed to capture complex relationships between alloy compositions, temperature, and mechanical properties. The effects of mechanical properties and temperature on alloy behavior were classified as positive or negative, providing a systematic framework for performance evaluation. The training process was carefully monitored to avoid overfitting, with statistical analyses conducted to validate data consistency. Comparisons between the ANN-predicted results and JMatPro-simulated values confirmed the robustness and accuracy of the proposed model.

To ensure the dataset's reliability and compatibility with the ML framework, the raw data obtained from JMatPro simulations underwent rigorous preprocessing. This included unit standardization, scaling, and statistical verification against the original dataset. These steps ensured that the model inputs were precise and consistent, yielding accurate predictions of mechanical properties. The resulting dataset, derived from CMS simulations, proved to be a robust source for training and validating the ANN model, demonstrating the effectiveness of integrating CMS and AI methodologies in alloy design and property prediction.

Simulation's Heat Treatment Conditions The simulations for this study were conducted using the JMatPro software, which is rooted in computational materials science principles. The software was utilized to model 50 unique compositions of Ni-Cr-Fe-based nickel alloys, with controlled proportions of elements such as Cr, Fe, Mo, and Al, among others. Heat treatment parameters were tailored to optimize the formation of gamma (γ), gamma prime (γ'), and gamma double prime (γ'') phases, which are critical contributors to the alloys' mechanical properties. As shown in Figure 2, the "Bimodal" distribution was selected for precipitate size, with γ' precipitates set at 10 nm and γ'' precipitates at 50 nm, ensuring realistic microstructural features. For each alloy composition, Time-

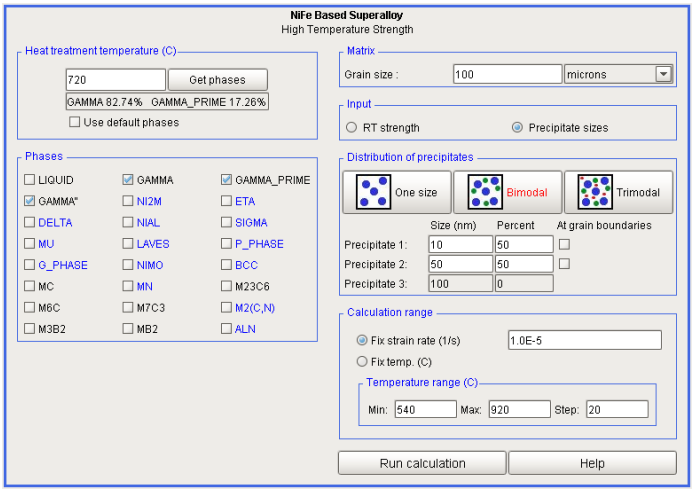

Figure 2 Input Parameters and Bimodal Distribution Settings for Ni-Cr-Fe Based Nickel Alloys Simulation in JMatPro

Temperature-Transformation (TTT) diagrams and Phase Fraction Diagrams were generated to determine the optimal heat treatment temperatures for forming the desired precipitates while avoiding deleterious phases such as delta, eta, and laves (Handbook 1991; Saunders 2010). These phases, known for their detrimental impact on mechanical properties, were excluded by simulating equilibrium conditions, ensuring that only phases relevant to practical processing conditions were considered. The grain size of the matrix phase was standardized at 100 microns, providing consistency across simulations.

Heat treatment simulations were conducted over a temperature range of 540°C to 920°C, reflecting operational conditions relevant to Ni-Cr-Fe alloys used in high-temperature applications (Francis *et al.* 1967). This range allowed a comprehensive evaluation of

mechanical properties, including 0.2% Proof Stress, Fracture Stress, and Young's Modulus. The parameters were optimized to promote complete precipitation of γ' and γ'' phases within the matrix, enhancing the strength and thermal stability of the alloys (Wu *et al.* 2022; Nembach and Neite 1985).

The simulation results provided detailed insights into the microstructural evolution and mechanical behavior of these alloys, offering a robust foundation for subsequent machine learning predictions. By focusing on γ' and γ'' precipitates, this study aligns with prior research that underscores their pivotal role in strengthening nickel-based superalloys (Smith *et al.* 2021; Liu *et al.* 2023).

Dataset Generation The generation of a comprehensive dataset is pivotal for the accurate modeling and prediction of the mechanical properties of Ni-Cr-Fe-based nickel alloys. These alloys are extensively utilized in high-temperature applications due to their exceptional mechanical performance, which can be enhanced through solution treatment and aging processes (Du *et al.* 2021). These heat treatment processes stabilize the microstructure, enabling the material to maintain its strength and integrity over prolonged periods, a feature that is critical in industries like aerospace and power generation (Vijayakumar *et al.* 2024). Precipitation hardening, facilitated by specific alloying elements, significantly enhances the strength of these alloys under elevated thermal conditions, making them ideal for nickel alloys applications (Zielinska *et al.* 2010).

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

The alloy compositions used in this study were systematically designed to optimize their mechanical properties. As outlined in Table 1, the primary elements Ni, Cr, Fe, Co, Mo, Nb, and Ti were varied within specific weight fractions, while secondary elements Al, Mn, Si, and Cu were held constant to maintain consistency in their precipitation hardening effects. Phase Fraction Diagrams and Time-Temperature-Transformation (TTT) Diagrams were generated using JMatPro for each composition to simulate their behavior under various thermal conditions. This approach allowed the modeling of 50 distinct alloy compositions, evaluated at 20 different temperatures ranging from 540°C to 920°C in 20°C increments, resulting in a total of 1000 data rows.

Table 2 presents an excerpt from the dataset, illustrating two alloy compositions. Notably, the second composition, which includes an additional 1% Co, demonstrates enhanced mechanical properties, highlighting the critical influence of individual alloying elements. This dataset captures 0.2% Proof Stress (MPa), Fracture Stress (MPa), and Young's Modulus (GPa) across varying temperatures, providing a robust foundation for analyzing the impact of thermal and compositional variations on the mechanical behavior of nickel alloys (Goodfellow *et al.* 2019). This structured dataset serves as a critical resource for understanding the relationships between alloy composition, heat treatment conditions, and resulting mechanical properties, aligning with recent advancements in nickel alloys research (Behera *et al.* 2024; Ju *et al.* 2024).

Development of the Artificial Intelligence Model The development of the proposed ANN model was designed to accurately predict the mechanical properties of Ni-Cr-Fe alloys, leveraging a dataset generated through Computational Materials Science (CMS) simulations. The dataset, consisting of 1,000 rows, was carefully preprocessed to ensure consistency and accuracy, including normalization of input features and handling missing data. The input features, such as elemental compositions and temperature, were scaled between 0 and 1 using Min-Max Normalization, ensuring that the model could efficiently process the data.

The ANN architecture was tailored to capture the complex nonlinear relationships between the input features and target properties (0.2% proof stress, fracture stress, and Young's modulus). It consisted of multiple hidden layers, each optimized to enhance the learning capacity of the model while avoiding overfitting. The model was trained using 80% of the dataset, with the remaining 20% allocated for validation and testing. To further enhance the model's robustness, the training process incorporated regularization techniques and monitored validation loss to prevent overfitting. The results demonstrated the model's ability to generalize effectively, providing accurate predictions across diverse alloy compositions and thermal conditions.

Artificial Neural Network Architecture The ANN architecture in this study was designed to predict the mechanical properties (0.2% proof stress, fracture stress, and Young's modulus) of Ni-Cr-Fe alloys with high accuracy. The network employs a multilayer architecture optimized for capturing the nonlinear and complex relationships between compositional and thermal input features and the target mechanical properties. The input layer includes 12 features, representing elemental compositions (e.g., Ni, Cr, Fe) and temperature, which are preprocessed using a standardization technique to ensure consistent scaling across all inputs.

The hidden layers of the network were constructed to maximize learning efficiency while preventing overfitting. The first hidden layer contains 512 neurons, followed by 256 neurons in the second hidden layer, and 128 neurons in the third. Each layer uses ReLU (Rectified Linear Unit) activation functions to introduce nonlinearity, while batch normalization improves convergence speed and training stability. Additionally, dropout regularization (40% in the first layer and 30% in subsequent layers) is employed to prevent overfitting by randomly deactivating a subset of neurons during training.

The output layer includes three neurons corresponding to the target properties. A linear activation function is applied in this layer to ensure continuous outputs. The network uses the Mean Squared Error (MSE) as the loss function to minimize prediction errors and the Adam optimizer for efficient weight updates during training. To enhance the model's generalization capability, early stopping and learning rate reduction techniques were incorporated, ensuring training halts when validation loss no longer improves.

This carefully designed architecture enables the ANN model to generalize effectively across diverse compositions and temperatures, making it a robust tool for predicting the mechanical properties of Ni-Cr-Fe alloys with minimal computational overhead.

RESULTS AND DISCUSSION

The experimental tests conducted for the proposed ANN model demonstrated its robust capability to predict the mechanical properties of Ni-Cr-Fe alloys with high accuracy. The model was trained and validated using a dataset generated through Computational Materials Science (CMS) simulations, which encompassed 0.2% proof stress, fracture stress, and Young's modulus as target mechanical properties. The training and validation loss curves revealed a smooth and rapid convergence, indicating that the model effectively learned the underlying relationships in the dataset with-

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

out overfitting. The alignment between actual and predicted values, as visualized in the evaluation graphs, confirmed the ANN model's ability to generalize and accurately predict material behavior across diverse compositions and temperature ranges.

Furthermore, the model's prediction errors were predominantly centered around zero, with narrow distributions for all three mechanical properties, especially for Young's modulus, which exhibited the least variability. This highlights the model's precision and reliability in predicting alloy stiffness, alongside its robust performance in estimating fracture and proof stress values. Additionally, the impact of individual input features, such as temperature and compositional elements, on the model's predictions provided critical insights. Temperature was identified as the most influential parameter, aligning with its dominant role in determining the mechanical performance of alloys. These findings demonstrate the potential of integrating CMS simulations with machine learning approaches to enhance the speed and accuracy of material design processes.

Performance of AI Model As shown in Table 3, the predicted mechanical properties (0.2% proof stress, fracture stress, and Young's modulus) for specific alloy compositions at 760°C are compared with the values obtained from JMatPro simulations. The accuracy percentages for each property demonstrate the effectiveness of the proposed ANN model in predicting mechanical behavior.

The fracture stress exhibits the highest accuracy, nearing 99.99%, followed by Young's modulus and 0.2% proof stress, both exceeding 94%. This high level of accuracy confirms the model's ability to generalize well, even for compositions outside the training dataset. Additionally, the minimal deviations between the predicted and simulated values indicate that the model is robust in handling diverse alloy compositions and conditions.

These findings emphasize the practical applicability of the model, particularly in predicting mechanical properties at 760°C, a temperature critical for high-performance applications. The results validate the ANN model as a reliable computational tool for optimizing alloy design and reducing the need for extensive experimental efforts.

As shown in Table 4, the performance of the proposed artificial neural network (ANN) model in predicting the mechanical properties of Ni-Cr-Fe alloys was assessed using three primary metrics: Mean Squared Error (MSE), Mean Absolute Error (MAE), and R-squared (R^2) Score. The MSE value of 296.7164 indicates the model's capability to minimize the squared differences between the predicted and actual values, reflecting its ability to provide consistent predictions. The MAE value of 11.6829 highlights the model's precision, showing that the average magnitude of prediction errors remains low across the test dataset. Furthermore, the R^2 score of 0.8899 demonstrates that the model accounts for 88.99% of the variance in the mechanical properties, confirming its robustness in modeling the complex relationships between compositional and thermal features. These results, as summarized in Table 4, validate the ANN model as an effective computational tool for accurately predicting mechanical properties, offering significant potential for alloy design and optimization applications.

Figure 3 illustrates the performance of the proposed artificial neural network (ANN)-based model in predicting the mechanical properties (0.2% proof stress, fracture stress, and Young's modulus) of Ni-Cr-Fe alloys. The horizontal axis represents the actual values, while the vertical axis shows the values predicted by the model. The close alignment of data points along the $y = x$ diagonal line demonstrates that the model predicts the actual values with high accuracy and without systematic errors. The three different mechanical properties are represented by distinct colors (blue: 0.2% proof stress, orange: fracture stress, green: Young's modulus). The strong linear relationship observed across all properties indicates that the ANN model effectively learned the relationships within the training data. Particularly, the fracture stress predictions, represented by the orange points, show remarkable accuracy across a wide range of values, highlighting the model's robust performance for this parameter. Similarly, high prediction accuracy was achieved for 0.2% proof stress and Young's modulus. The model

Table 3 Accuracy Rates of Predicting the Mechanical Properties of the Alloy Composition Determined Outside the Dataset at 760 °C Using the AI Model.

Composition (wt%)	Mechanical Properties	JMatPro	AI Model	Accuracy (%)
Ni: 61%, Ti: 2.5%, Cr: 20%, Al: 0.5%, Fe: 6%, Mn: 1%, Co: 0%, Si: 0.5%, Mo: 3%, Cu: 0.5%, Nb: 5%	0.2% Proof Stress (MPa)	809.53	881.23	91.143
	Fracture Stress (MPa)	1517.01	1516.98	99.998
	Young's Modulus (GPa)	152.49	159.21	95.593
	Overall Accuracy (%)			95.578
Ni: 65%, Ti: 2.5%, Cr: 18%, Al: 0.5%, Fe: 8%, Mn: 1%, Co: 1%, Si: 0.5%, Mo: 2%, Cu: 0.5%, Nb: 1%	0.2% Proof Stress (MPa)	561.3	590.21	94.849
	Fracture Stress (MPa)	1216.77	1181.13	97.070
	Young's Modulus (GPa)	156.64	152.90	97.612
	Overall Accuracy (%)			96.510
Ni: 63.5%, Ti: 1%, Cr: 16%, Al: 0.5%, Fe: 10%, Mn: 1%, Co: 2%, Si: 0.5%, Mo: 0%, Cu: 0.5%, Nb: 5%	0.2% Proof Stress (MPa)	649.83	654.59	99.267
	Fracture Stress (MPa)	1405.87	1322.45	94.066
	Young's Modulus (GPa)	155.74	155.78	99.974
	Overall Accuracy (%)			97.769
Average Accuracy Rate				96.619

Table 4 Evaluation of the Artificial Neural Network (ANN) Model Performance Metrics: Mean Squared Error (MSE), Mean Absolute Error (MAE), and R-squared (R^2) Score.

Metric	Value
Mean Squared Error (MSE)	296.7164
Mean Absolute Error (MAE)	11.6829
R-squared (R^2) Score	0.8899

was trained on a dataset of 1000 rows generated using CMS (Computational Materials Science) simulations and achieved high accuracy rates (over 95%) on test and validation datasets. This result demonstrates the ANN model's capability to effectively capture the complex compositional and temperature-dependent relationships of Ni-Cr-Fe alloys, supporting the reliability of the proposed methodology. These findings align with the overall results of the study and underscore the efficacy of integrating CMS-generated datasets with AI models, offering significant time and cost advantages compared to experimental approaches. Consequently, the graph highlights the practical potential of the proposed model in advancing alloy design and optimization.

As shown in Figure 4, this chart illustrates the relative importance of input features in predicting mechanical properties using the proposed ANN model. The x-axis represents the importance scores, while the y-axis lists the input features, including temperature and elemental compositions. Among the features, temperature (°C) stands out as the most influential factor, indicating its dominant role in determining the mechanical properties of Ni-Cr-Fe alloys. Elements such as Ti, Nb, and Ni exhibit moderate importance, while elements like Cu, Si, and Mn have minimal impact. These results emphasize the critical role of temperature and specific elements in alloy design and optimization processes and demonstrate the ANN model's ability to accurately capture

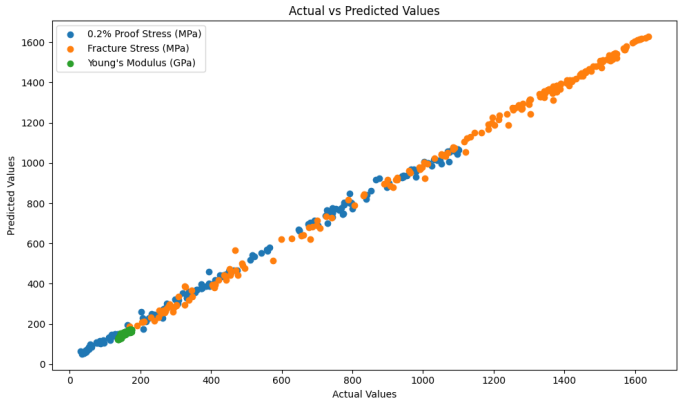

Figure 3 Comparison of Actual and Predicted Mechanical Properties: 0.2% Proof Stress, Fracture Stress, and Young's Modulus

these complex interactions.

As shown in Figure 5, this correlation matrix illustrates the relationships among the input features (elemental compositions and temperature) and the mechanical properties (0.2% proof stress, fracture stress, and Young's modulus) in the proposed model. The color scale represents the strength and direction of the correlation, with dark red indicating strong positive correlation (+1.00) and dark blue indicating strong negative correlation (-1.00). The matrix reveals strong negative correlations between temperature and Young's modulus (-0.98), 0.2% proof stress, and fracture stress (-0.76), highlighting the decline in mechanical properties with increasing temperature. Among the elemental compositions, a notable negative correlation is observed between Ni and Cr (-0.57), while Cr and Ti exhibit a positive correlation (+0.30). Additionally, strong positive correlations are observed between mechanical properties, such as 0.2% proof stress and fracture stress (+0.95).

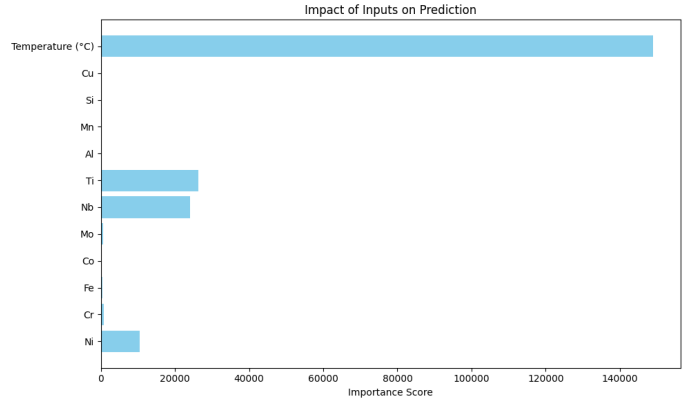

Figure 4 Impact of Input Features on Prediction: Relative Importance of Temperature and Elemental Compositions

This matrix underscores the complex interdependencies between input features and mechanical properties effectively captured by the model.

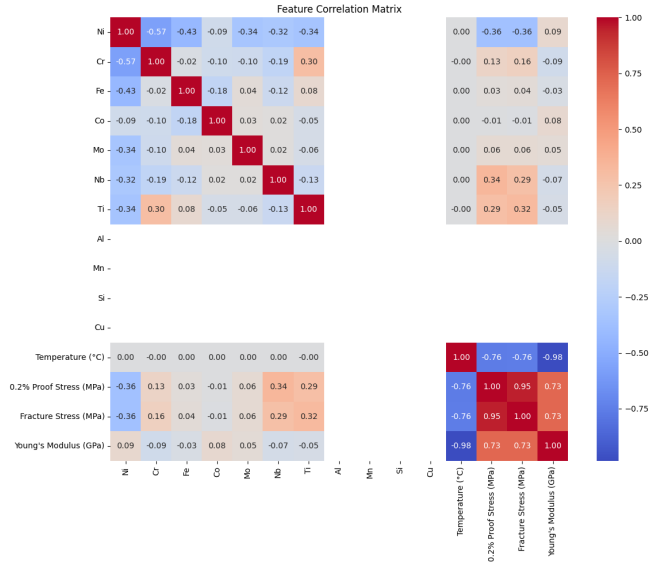

Figure 5 Analysis of Correlations Between Input Features and Mechanical Properties: Effects of Temperature and Compositions

As shown in Figure 6, the predicted mechanical properties (0.2% proof stress, fracture stress, and Young's modulus) of three new alloys (Alloy 1, Alloy 2, and Alloy 3) are presented for comparison. The x-axis represents the different alloys, while the y-axis indicates the predicted values for each mechanical property. Among the properties, fracture stress (orange bars) shows the highest values across all three alloys, highlighting their strong resistance to fracture. Alloy 1 exhibits the highest fracture stress, outperforming Alloy 2 and Alloy 3 in terms of overall durability. Similarly, 0.2% proof stress (blue bars) is slightly lower but consistent among the three alloys, with Alloy 1 again showing a marginally higher value, indicating its superior resistance to elastic deformation. Young's modulus (green bars), representing stiffness, is the lowest among the three properties and displays minimal variation between the alloys. This suggests that the stiffness of these alloys remains relatively constant despite differences in fracture and proof stress. Overall, Alloy 1 demonstrates the best mechanical performance, particularly in fracture stress and proof stress, making it the most durable of the three new alloys.

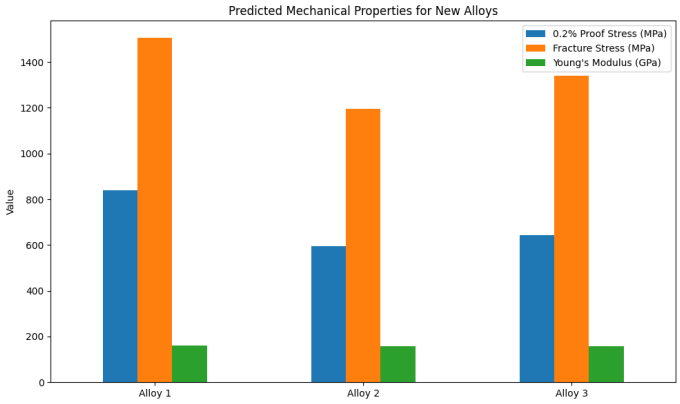

Figure 6 Predicted Mechanical Properties for New Alloys

As shown in Figure 7, this graph illustrates the error distributions of the predicted values for 0.2% proof stress (blue), fracture stress (orange), and Young's modulus (green). The x-axis represents the error values, while the y-axis shows the frequency of predictions within those error ranges. The error distributions for all three properties are centered around zero, indicating that the model is unbiased and provides accurate predictions. Among the distributions, Young's modulus (green) exhibits the narrowest range, suggesting higher precision for this property compared to the others. In contrast, fracture stress (orange) has a slightly wider distribution, indicating greater variability in its predictions. Despite this, the errors remain concentrated around zero for all properties, highlighting the robustness of the model. The near-symmetry of the distributions confirms that the model neither systematically overestimates nor underestimates the values. A few outliers exist at the extreme ends, but their frequency is minimal, demonstrating that large errors are rare. Overall, the model achieves reliable and consistent predictions for all mechanical properties, with particularly strong performance in predicting Young's modulus.

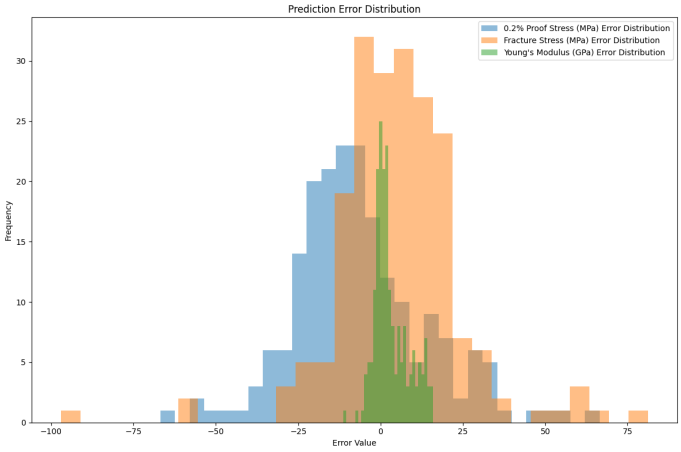

Figure 7 Training and Validation Loss Progression Across 500 Epochs for the Proposed ANN Model

As shown in Figure 8, this graph illustrates the progression of training loss (blue line) and validation loss (orange line) for the proposed ANN model over 500 epochs. The x-axis represents the number of epochs, while the y-axis shows the loss values, which indicate the error in the model's predictions. Both training and validation losses start at high values and decrease significantly during the initial phase, particularly in the first 100 epochs, demonstrating the model's ability to learn and reduce prediction errors effectively. After approximately 200 epochs, the losses converge to similar values, with both training and validation loss stabilizing near zero, indicating that the model has achieved a high level of accuracy and generalization. The lack of divergence between the two curves suggests that the model does not overfit the training data, as the validation loss closely follows the training loss throughout the process. This smooth and consistent convergence highlights the robustness of the model and the effectiveness of the training procedure in minimizing errors while maintaining good performance on unseen data. Overall, the graph confirms the reliability and efficiency of the ANN model in learning the complex relationships within the dataset.

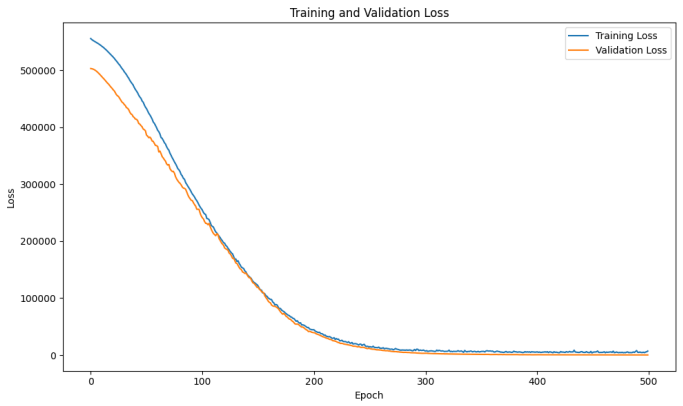

Figure 8 Training and Validation Loss Progression Across 500 Epochs for the Proposed ANN Model

The results of this study demonstrate the effectiveness of integrating Computational Materials Science (CMS) simulations and artificial intelligence, specifically artificial neural networks (ANNs), in predicting the mechanical properties of Ni-Cr-Fe alloys. The high accuracy of the ANN model, validated by its strong alignment with simulation data and minimal prediction errors, highlights its potential as a reliable computational tool for alloy design. By accurately predicting 0.2% proof stress, fracture stress, and Young's modulus across various compositions and temperatures, the model addresses the challenges of experimental limitations, such as time-consuming procedures and high costs.

The model's ability to generalize well to unseen compositions was confirmed by its performance on test datasets, where prediction errors were centered around zero with limited outliers. Furthermore, the correlation matrix analysis revealed the dominant role of temperature in determining mechanical properties, alongside significant contributions from specific elemental compositions like Ti, Nb, and Ni. This aligns with prior studies that emphasize the importance of temperature and compositional effects on material behavior.

This approach provides a scalable alternative to traditional experimental methods, allowing rapid exploration of compositional spaces and optimization of material properties for high-performance applications. The study underscores the potential of combining CMS-generated datasets with machine learning to accelerate material development, reduce dependency on costly experiments, and improve the precision of alloy design processes. Future work may focus on expanding the dataset to include additional compositions and thermal conditions, further enhancing the model's predictive capabilities and applicability in diverse industrial contexts.

CONCLUSION

The findings of this study demonstrate the effectiveness of integrating Computational Materials Science (CMS) simulations with artificial neural networks (ANNs) for predicting the mechanical properties of Ni-Cr-Fe alloys. The proposed ANN model achieved high accuracy in estimating 0.2% proof stress, fracture stress, and Young's modulus across diverse alloy compositions and temperatures, as validated by metrics such as a low Mean Squared Error (MSE) of 296.7164 and a high R-squared (R^2) score of 0.8899. These results confirm the model's capability to capture complex nonlinear relationships between input features and target properties, making it a valuable computational tool for alloy design and optimization.

One of the key advantages of this approach is its ability to minimize the dependency on time-consuming and expensive experimental procedures. By leveraging CMS-generated datasets, the model provides rapid and reliable predictions, enabling efficient exploration of large compositional spaces. The high generalization capability of the ANN model further supports its application in real-world scenarios, particularly in industries requiring high-performance materials, such as aerospace, energy, and automotive sectors.

Future work could focus on expanding the dataset to include additional alloy compositions, broader temperature ranges, and other critical properties to enhance the model's applicability. Additionally, exploring advanced machine learning techniques, such as ensemble learning or transfer learning, may further improve predictive accuracy. The integration of experimental validation with machine learning predictions could also provide a comprehensive framework for advancing material science research. Overall, the study highlights the potential of AI-driven approaches in accelerating material design, reducing costs, and achieving more precise predictions in alloy development.

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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