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Machine learning-based prediction of surface roughness and machinability in heat-treated Ni–Cr–Mo low-alloy steels

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ABSTRACT

Nickel–chromium–molybdenum (Ni–Cr–Mo) low-alloy steels are commonly used in automotive and aerospace industries for their strength and fracture toughness. However, these steels are difficult to machine. Their poor machinability often results in rapid tool wear, a poor surface finish, and higher production costs. To address these challenges, this study integrates tailored and novel heat treatment processes with machine learning models to predict machining performance. Two heat treatment procedures were examined: conventional isothermal annealing (ITA), which generates a heterogeneous pearlite–ferrite–bainite structure, and a novel multi-step process [Normalized Subcritical Annealing (NSA)], designed to refine the microstructure into a uniform pearlite–ferrite–carbide matrix with reduced hardness variation. Mechanical properties, including yield strength, ultimate tensile strength, elongation, reduction in area, proof stress, Young's modulus, and impact energy, were measured and used as input features. Several regression models, including random forest, XGBoost, ridge, support vector regression, K-nearest neighbors, a stacking regressor, and a multilayer perceptron, were trained to predict two machining outcomes: surface roughness (Ra) and machinability index (%). The results indicate that impact energy and yield strength serve as the most influential features, establishing a direct correlation between toughness and strength in relation to machining performance. Heat treatment-dependent trends were observed. For ITA samples, random forest captured the machinability index more effectively, reflecting the broader property distributions of the heterogeneous microstructure. For NSA samples, random forest provided better predictions of surface roughness "Ra," consistent with the uniformity of the refined structure. However, the coefficient of determination (R^2) was moderate. The models demonstrated high predictive precision with strong industrial relevance, as evidenced by their low error metrics. This accuracy can often be more valuable for industrial decision-making than simply achieving a perfect fit. This study is the first to establish a data-driven link between a novel NSA heat treatment and machine learning predictions for machining outcomes. Overall, NSA treatment is best suited when a consistent surface finish is required, while ITA provides flexibility in tuning machinability, providing practical guidelines for industrial applications. The findings provide a framework that supports alloy design and optimizes machining processes, reducing reliance on trial-and-error methods.

I. INTRODUCTION

The automotive and aerospace sectors use materials that are strong, long-lasting, and easy to process. Ni–Cr–Mo low-alloy steels are often selected for critical aerospace and automotive components such as gears, shafts, and bearings.[1] These steels combine low weight with high strength, toughness, and fatigue resistance. This helps improve performance and extends part life.[2] They also offer good mechanical strength and can resist wear and corrosion.[3] However, their high strength makes them difficult to machine. Standard machining methods struggle with these steels.[4] Tools wear out quickly, and the surface finish often suffers. As tool wear increases, the quality of the surface goes down.[5] Flaws on the surface can lead to cracks or oxidation, which reduce the part's reliability and result in higher production costs.[6]

To solve these problems, both the material and the machining process need to be improved.[7] One method is to add elements such as sulfur, lead, or bismuth. These help with machining but can weaken the steel or raise environmental concerns. Heat treatment is another viable option. It changes the steel's internal structure and can make it easier to machine. Heat treatment is key to controlling the structure and strength of these steels. Steps such as quenching and tempering adjust the grain size, phase, and hardness. When done correctly, these steps give a good balance of strength, toughness, and wear resistance. This is important for parts used in cars, aircraft, and energy equipment. The heat treatment process must be accurate to get the best results.[8,9] The process involves heating and cooling the steel in a controlled way to get the right properties.[10] Traditional methods depend on previous experience and trial runs, but these approaches do n't always yield effective results.

Machinability refers to the ease with which a material can be shaped to achieve the desired size and finish. It depends on factors such as hardness, grain structure, chemical composition, and cutting conditions. In Ni–Cr–Mo low-alloy steels, even slight changes in grain size or precipitates can significantly impact how the material cuts. These changes can wear tools out faster and leave a poor surface finish.[11] Traditional machinability tests are complex, slow, and costly. They may also miss how structure affects machining. Regular machining techniques are often not cost-effective for Ni–Cr–Mo low-alloy steels.[12] Machinability is also influenced by factors such as cutting speed, feed, depth of cut, and tool shape. However, internal steel properties play a significant role. Due to these complex factors, optimizing the machining of Ni–Cr–Mo low-alloy steels is difficult.

Previous research has focused on understanding the alloying effects, machining challenges and ductile-to-brittle transition in Ni–Cr–Mo low-alloy steels. For example, DelRio *et al.* (2020) examined how tempering temperature influences fracture behavior.[13] Newer methods such as electrochemical machining have also been shown to improve efficiency, reduce tool wear, and provide better precision than conventional techniques.[14] Liu *et al.* linked Ni and Mo contents to grain refinement and cryogenic toughness.[15] Sousa *et al.* highlighted the impact of minor compositional changes from recycled steel on machinability and found that small differences in Ni, Cr, and Cu levels from recycled steel affected machinability.[16] Pratomo *et al.* showed the role of nickel in refining grains and enhancing machinability without compromising impact toughness.[17]

The findings from previous studies align closely with the goals of the present work. This work emphasizes the importance of optimizing heat treatment to balance strength and toughness.[18,19] This supports the tailored heat treatment approach developed in the present work. The process enhances microstructural uniformity while maintaining mechanical performance. Electrochemical machining and nanocomposite coatings improve tool life and surface finish.[20,21] This study aims to achieve similar goals by reducing hardness variations and enhancing machinability.

Furthermore, the growing shift toward data-driven machinability assessment aligns with the present work's application of machine learning (ML) models, which provide predictive insights into machining performance.[22] Together, these advancements emphasize the importance of combining innovative heat treatment processes for microstructure control with intelligent predictive modeling to enhance manufacturing results. The present work builds on these advances by moving beyond conventional heat treatment studies and empirical machinability tests. The novelty of this research lies in combining the mechanical properties derived from novel heat treatment processes with machine learning-based predictions in Ni–Cr–Mo low-alloy steels. This approach precisely forecasts distinct trends in machinability associated with conventional and novel multi-step heat treatments. Additionally, it identifies impact energy and yield strength as key predictive features, providing physically direct relationships between mechanical properties and machining behavior. Together, these contributions establish a new, data-driven approach for machining optimization and alloy design.

Machine learning (ML) aids in analyzing large datasets to identify patterns and predict machining outcomes. Models such as random forests and deep neural networks can predict machinability based on material properties and cutting data.[23] These models are trained using experimental results, thereby improving efficiency and reducing the need for physical testing. ML algorithms are strong tools for prediction and process optimization in materials and manufacturing. Supervised ML identifies complex relationships between processing steps, material content, and properties such as machinability or hardness.[24] Neural networks and support vector machines are well-suited for nonlinear data and can make accurate predictions in treatment settings.[25] ML uses "descriptors," numerical values representing material features, for fast screening and prediction.[26] These help with computational analysis and make the data usable for ML models.[27] In manufacturing, ML enables the development of innovative and intelligent systems that automatically adjust to correct errors in real-time.[28]

Predictive models help determine optimal cutting settings, extend tool life, and reduce defect rates. A recent method combines structural and mechanical data of Ni–Cr–Mo low-alloy steels with ML tools.[29] This bridges metallurgy and manufacturing to enhance strategies for machining difficult-to-machine materials. Merging ML into manufacturing boosts productivity, lowers waste, and improves quality.[30]

Surface roughness and the machinability index serve as crucial indicators of a material's ability to undergo effective and efficient machining. Understanding these concepts helps achieve better quality and more efficient results. Traditional testing methods are slow and costly, and they often fail to effectively capture the influence of microstructure and mechanical properties. Predicting these outcomes in advance is, therefore, essential to minimize trial-and-error, reduce material and tooling costs, and guide the selection of heat treatment for better performance.

This study is motivated by the need to reduce machining costs, extend tool life, and enhance production efficiency in addressing the machinability challenges of Ni–Cr–Mo steels. Conventional machinability tests are time-consuming and costly, and often fail to accurately capture the influence of microstructure and mechanical properties on machining performance. Predicting outcomes, such as surface roughness and the machinability index, in advance can reduce reliance on trial-and-error machining. By linking heat treatment-induced mechanical properties with machine learning predictions, this work provides a practical, data-driven framework for selecting heat treatment routes [isothermal annealing (ITA) vs Normalized Subcritical Annealing (NSA)] that optimize machining behavior and reduce cost.

With data from heat-treated samples, ML predicts surface roughness and the machinability index.[31] It links traits such as strength, elongation, and grain size to machining results. This reduces the need for physical testing and speeds up analysis.[32,33] This study builds on that concept. It uses regression models trained on structural and mechanical inputs. The model accurately predicts machinability and surface quality. It also identifies key factors affecting machining. We used scanning electron microscopy images and test data from both conventional and modified heat treatments of Ni–Cr–Mo low-alloy steel. The models show that grain size, ductility, and strength ratios have a substantial impact on machining behavior. This method moves away from trial-and-error and supports prediction-based machining. It improves decision-making, product quality, and resource efficiency. Hence, machine learning is a key tool in advancing precision, productivity, and cost-effectiveness in smart and intelligent manufacturing.

II. MATERIALS AND METHODOLOGY

A. Materials and heat treatment

This study used rolled Ni–Cr–Mo low-alloy steel bars with a diameter of 90 mm. The exact chemical composition of the steel was determined using optical emission spectroscopy, and the results are presented in Table I. As mentioned above, these steel grades are used in the manufacture of automotive and aerospace components, including gears, shafts, and bearings. These materials are designed to provide exceptional strength and durability, making them ideal for high-performance situations where resilience is critical. Their toughness and ability to withstand fatigue can pose challenges during machining, as achieving a smooth finish is often tricky due to their hardness, and cutting tools tend to wear out more quickly. Therefore, careful planning and precise execution are vital during manufacturing to maintain high quality and efficiency.

Two distinct heat treatment techniques were employed to investigate how changes in the microstructure impact the machinability of the steel. The first approach was a standard isothermal annealing process, where the samples were heated to 960 °C until they entirely transformed into a uniform austenitic phase. After that, they were moved to a furnace maintained at 635 °C and held there for 7 h to allow the steel to transform fully. Once done, they were cooled to room temperature in the air. From this point onward, this standard process is designated as ITA. This traditional method yielded a mixed and heterogeneous microstructure, characterized by bands of pearlite and ferrite, along with patches of bainite or martensite in specific areas. These differences in the microstructure caused the hardness to vary significantly across the sample, making the material less ideal for even machining.

To address some of the challenges faced with previous methods, we developed a novel multi-step heat treatment process called NSA. This approach involves three key stages carried out in a specific order: normalizing with forced air cooling, subcritical annealing, and step tempering. First, the samples are heated up to 960 °C, which makes the steel structure uniform by dissolving carbides and transforming them into austenite. Immediately after, they are cooled quickly in the air to refine the grain structure and ensure consistency across the sample. The final stage involves holding the samples at 690 °C, a temperature below the critical point, to encourage a fine mixture of pearlite and ferrite. This step helps carbon and other alloying elements to spread evenly, reducing differences in hardness and making the material more uniform overall.

In the final stage, the samples were tempered in two steps: first at 650 °C and then at 600 °C, with the total tempering time kept equivalent to that of the conventional ITA process. The NSA treatment produced a homogeneous pearlite–ferrite–carbide matrix with much lower hardness variation across the cross section. The differences between the ITA and NSA microstructures were verified using optical microscopy and hardness mapping, which confirmed that the NSA route yielded a refined and stable microstructure favorable for machining applications.

In this study, we carefully measured several mechanical and machining properties of both ITA and NSA samples. We looked at different properties of the material to understand its behavior better. These included the amount of force it can withstand before breaking, its stretchability, and how it responds under impact. We selected these qualities because they provide a comprehensive overview of the material's strength, flexibility, stiffness, and toughness. All of these factors are important when figuring out how easy it will be to work with the alloy. The information gathered from these tests will help us develop more accurate predictions about how the material will perform in various situations.

B. Material characterization

Microstructural analysis was performed using an optical microscope (Olympus, Japan) to study phase distribution and grain morphology. Microhardness was measured using a Vickers tester (VMT-X, Matsuzawa, Japan) at a 0.05 kgf load for 10 s, with multiple indentations made across each sample to assess the hardness variation and uniformity. Tensile properties, yield strength, ultimate tensile strength (UTS), elongation, and reduction in area, were determined using a universal testing machine (UTE-60, FIE, India). Charpy V-notch impact tests were carried out on an AIT-300-N impact tester (Meta-test, India) to measure toughness. The surface finish was evaluated on machined samples using a surface profilometer (MicroXAM-800, KLA Corp., USA), with *Ra* values recorded for

TABLE I. Elemental composition of Ni–Cr–Mo low-alloy steels.

Elements	C	Mn	Si	Cr	Ni	Mo	Cu	Al	P	S
Wt. %	0.23	1.04	0.12	1.18	1.19	0.18	0.009	0.016	0.014	0.028

assessing machinability. All tests were conducted on both ITA- and NSA-treated samples for direct comparison.

C. Machine learning workflow

The mechanical properties of steel samples after treatment with conventional ITA and novel NSA processes were collected. Furthermore, it examines the effect of heat treatment processes on the machining characteristics of steel samples. The collected data were used to create and assess ML models that predict two key aspects of machining: surface roughness, which relates to the smoothness of the finished surface, and the machinability index, which reflects how easily the steel can be machined compared to standard free-cutting steels. Gaining a better understanding of this helps identify improved methods for working with these materials, leading to better quality and efficiency in manufacturing. Together, these outcomes represent critical metrics for evaluating and optimizing machining efficiency.

To develop dependable ML predictive models, we considered several key features, including yield strength (YS, MPa), ultimate tensile strength (UTS, MPa), 0.2% proof stress (MPa), elongation (% EL), reduction in area (% RA), the ratio of yield strength to ultimate tensile strength, Young's modulus (GPa), and impact energy (Joule). The expected outcomes were calculated based on engineering principles, and some natural randomness was added to reflect the variability typically seen during real-world machining processes. By formulating the problem in this way, the framework accounted for both the intrinsic variability of materials and the nonlinear relationships between mechanical properties and machining outcomes.

A variety of different regression methods were used to make sure that the specific behaviors for each task were accurately captured. The models tested included random forest, XGBoost, ridge regression (RR), support vector regression (SVR), K-nearest neighbors (KNNs), stacking regressor (an ensemble of multiple models), and a neural network-based Multilayer Perceptron (MLP). This diverse selection allowed comparison between linear, nonlinear, ensemble, and neural approaches. We divided the data so that 80% was used for training the model and the remaining 20% was used for testing its performance. To assess the accuracy of our predictions, we examined standard measures, including the average deviation from our predictions, the variation in predictions, and the model's ability to explain the overall variation in the data.

To make our analysis more reliable, we tested four different methods for preparing the data: using the raw inputs as they are, creating engineered features, removing outliers using a z-score method, and combining engineered features with filtering. We carefully tuned our model settings, crafted features, and validated our results to find the best combination for each machining target. All of this was done using Python 3.11, with tools such as Pandas and NumPy to handle the data, scikit-learn for building the models, and Matplotlib and Seaborn to create visualizations. This systematic workflow enabled the identification of heat treatment-specific and target-specific modeling strategies. For example, while NSA-treated samples yielded high-precision predictions for surface roughness, ITA-treated samples exhibited more reliable trends in machinability.

The heat treatment experiments, combined with machine learning models, helped us understand how the microstructure of Ni–Cr–Mo low-alloy steels influences their strength and how easily they can be machined and shaped.

D. Justification of machine learning models

This study used multiple regression models to analyze both linear and nonlinear relationships between mechanical properties and machining outcomes.

(a) Random forest (RF) is a widely used method due to its reliability in providing key influencing factors even in the presence of noisy experimental data. It is reliable for capturing complex non-linear interactions and clearly indicates which features are influencing factors. The RF is widely used in machining studies for predicting tool wear and surface finish because of its robustness against noisy experimental data.
(b) XGBoost was selected for analysis due to its better performance in handling structured data and its ability to model complex feature interactions. Its efficiency and embedded regularization mechanisms effectively manage complex feature interactions, thereby reducing overfitting in moderately sized datasets.
(c) Ridge Regression (RR) is a linear baseline model to correlate the properties. This model helps limit the size of coefficients, making predictions more stable by incorporating well-known correlations among mechanical properties. It is a valuable way to enhance the reliability of the results.
(d) Support Vector Regression (SVR) was employed to model potential non-linear relationships using kernel functions. This method illustrates how even minor or abrupt variations in mechanical properties, such as toughness and ductility, can substantially impact machining behavior. It is advantageous for comprehending threshold effects.
(e) K-Nearest Neighbors (KNNs): As an instance-based learning method, KNN helps in identifying local patterns. Its predictions are based on property similarity, which can reveal clusters of samples with comparable machinability.
(f) Stacking Regressor: This combines predictions from RF, XGBoost, and ridge models to improve accuracy across different material conditions, including both ITA and NSA datasets of this case.
(g) Multi-layer Perceptron (MLP): This neural network was tested to model highly complex, nonlinear functions that likely govern the interactions of multiple mechanical properties affecting machining outcomes.

Using this wide range of machine learning models enables a comprehensive comparison of ML algorithms, ensuring balanced conclusions that are not influenced by any single approach.

III. RESULTS AND DISCUSSION

The machine learning model predicts surface roughness and machinability in two different samples of Ni–Cr–Mo low-alloy steels: one treated with a proposed novel heat treatment, designated as "NSA," and the other with a regular and conventional heat

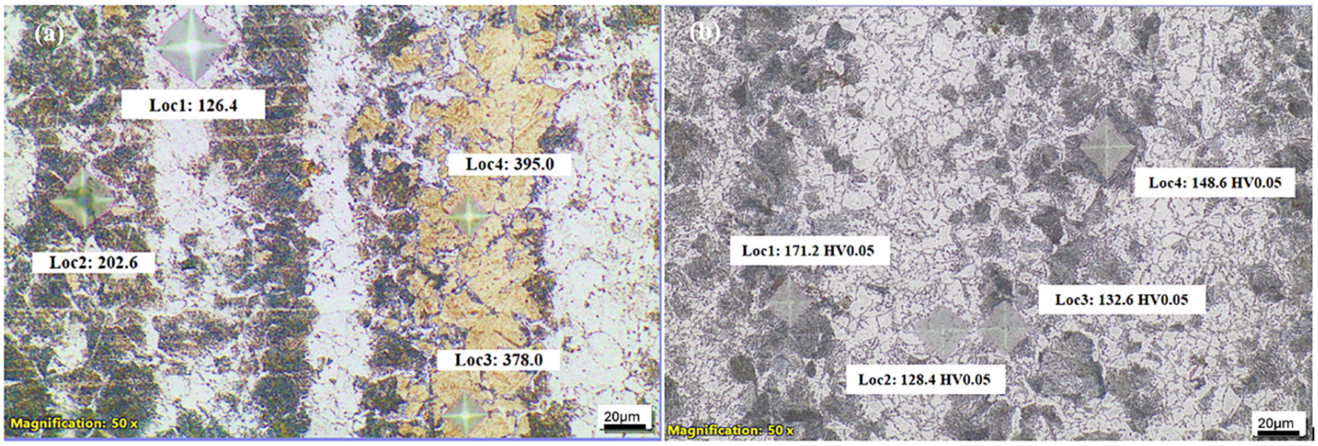

FIG. 1. Optical micrographs showing micro-hardness distribution of Ni–Cr–Mo low-alloy steel after two different heat treatments: (a) conventional isothermal annealing (ITA), which produces a banded pearlite–ferrite structure with significant hardness variation ranging from ∼192 to ∼373 HV, and (b) the novel multi-step heat treatment (NSA), which yields a refined and uniform pearlite–ferrite–carbide matrix with reduced hardness variation in the range of ∼132 to ∼173 HV. The NSA route clearly demonstrates improved microstructural uniformity and stability compared to the ITA process.

treatment process, defined as "ITA." Our models use basic mechanical properties to make fast and accurate predictions.

In microstructural and hardness distribution analysis, Fig. 1 shows the effect of ITA and NSA heat treatments on the microstructure and hardness distribution of Ni–Cr–Mo low-alloy steels. The ITA route yielded a banded pearlite–ferrite structure with bainite/martensite regions, leading to significant hardness variations across the sample (192–373 HV). Such heterogeneity introduces local differences in cutting resistance and tool loading, which, in turn, cause fluctuations in machinability. In contrast, the NSA treatment refined the microstructure into a uniform pearlite–ferrite–carbide matrix with much lower hardness variation (132–173 HV). This uniformity supports more stable chip formation and consistent surface finish during machining.

The differences observed in hardness distribution directly explain the modeling results reported in Table II. The greater variability in ITA properties created broader feature distributions, enabling random forest to identify non-linear trends in machinability. Conversely, the uniform structure of NSA reduced property variability, leading to precise predictions for surface roughness (*Ra*) but weaker trends in machinability, as reflected in the low R^2 and low root-mean-square error (RMSE) values. Thus, Fig. 1 provides the experimental evidence linking microstructural uniformity to the treatment-dependent predictive behaviors captured by the machine learning models.

A. Performance importance analysis

Engineers can select the appropriate heat-treated samples to get better machining performance without trial and error.

Surface roughness and machinability index were predicted separately for both heat-treated samples. Different machine learning models were tested to find the most accurate one. These included random forest, XGBoost, support vector regression, K-nearest neighbors, ridge regression, stacking regressor, and a type of neural network known as multi-layer perceptron. Each model was to assess its ability to predict the results based on the material properties. Figure 2 shows the predictive performance of machine learning models for two important machining outcomes, surface roughness ("Ra"), and machinability index (%). It was evaluated for two heat-treated samples: ITA and NSA. Using actual vs predicted scatterplots, each case was analyzed to understand the model's trends, accuracy, and limitations.

The predictive performance of different machine learning models for ITA and NSA samples is summarized in Table II. The same features were used for both the ITA and NSA datasets.

TABLE II. Predictive model performance matrix for ITA and NSA samples.

Heat treatment type	Target (machining outcomes)	Best model	R^2 score	Mean absolute error (MAE)	RMSE	Interpretation
Regular "ITA"	Surface roughness (*Ra*)	XGBoost	∼0.098	0.395	0.495	Moderate accuracy, weak trend
	Machinability index (%)	Random forest	∼0.201	0.825	0.996	Usable, strong trend
NSA	Surface roughness (*Ra*)	Random forest	0.035	0.0159	0.0200	High precision
	Machinability index (%)	Stacking regressor	−0.002	1.205	1.484	Weak feature

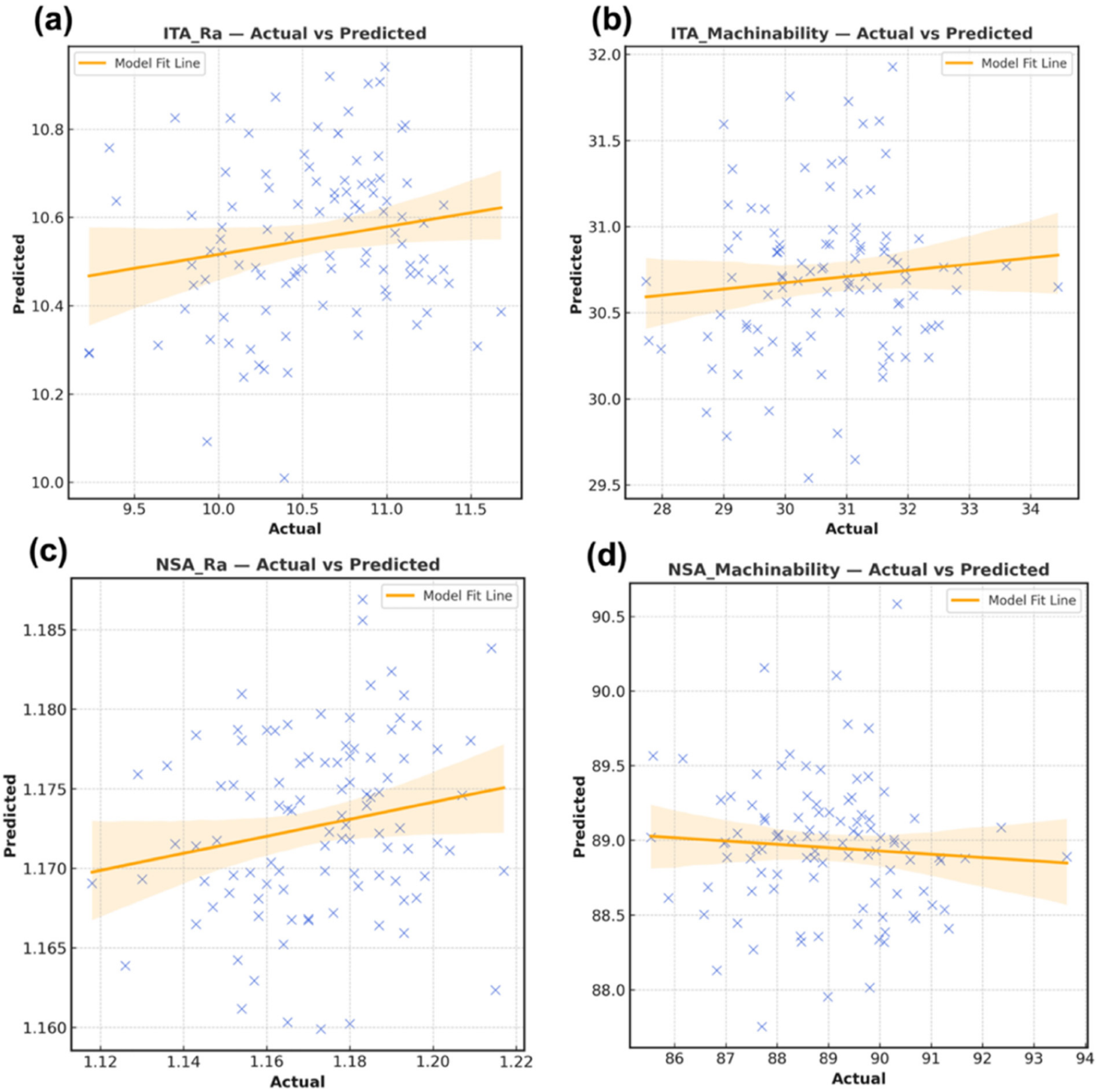

FIG. 2 Actual vs predicted plots for two machining outcomes—surface roughness (Ra) and machinability index, across two heat-treated samples, regular (ITA) and novel (NSA) treatments. (a) Surface roughness "Ra" for "ITA" sample using XGBoost regressor; (b) machinability index for ITA using random forest; (c) surface roughness "Ra" using random forest; (d) machinability index for NSA using stacking regressor. The orange line represents the model fit, with shaded areas indicating confidence intervals. Plots illustrate varying predictive accuracy across sample data and machining outcomes targets, highlighting the importance of task-specific modeling.

Differences in model performance are likely due to inherent statistical variations in these features, which represent the microstructures resulting from two different heat treatment processes.

The performance of the models in this study closely aligns with their designed functions. Random forest, with its robustness to noise and ability to highlight feature importance, performed best for machinability predictions in ITA-treated samples, where clear patterns of property and machinability were present. XGBoost, designed for structured data and strong non-linear fitting, gave moderate yet useful results for surface roughness predictions in ITA. In NSA-treated samples, where the microstructure was more uniform but less predictable, simple models struggled, and ensemble methods such as the stacking regressor or neural approaches like MLP were needed to capture subtle feature interactions. These outcomes reinforce the decision to employ a diverse set of models, each suited to specific material-treatment conditions and machining targets. The best-performing model for each scenario was selected based on RMSE (error size) and R^2 (fitting trend) metrics.

The results in Table II show no single model excelled across all machining targets and treatments. For ITA samples, random forest performed better in predicting the machinability index. This outcome can be attributed to the heterogeneous microstructure generated by ITA, which contains pearlite–ferrite bands along with bainitic/martensitic regions. Such heterogeneity introduces strong, nonlinear, yet discernible trends between toughness, strength, and machinability. Random forest, with its ability to capture non-linear interactions while maintaining robustness to noise, was, therefore, well-suited to these data.

In contrast, NSA samples, which exhibited a refined and more uniform microstructure, posed a different modeling challenge. The homogeneity of NSA decreased the variability in key mechanical properties, such as hardness, ductility, and toughness. This limited variation meant that simple decision-tree models alone could n't gather enough information for accurate machinability predictions, resulting in poor performance with random forest.

Figure 3 illustrates a conceptual schematic that links heat treatment, feature distributions, model choice, and prediction performance. ITA's heterogeneous microstructure favors random forest for machinability, while NSA's uniform structure requires ensemble models for machinability but enables random forest to give precise surface roughness predictions. In NSA samples, the predictive behavior differed significantly. For "Ra," Random forest achieved a very low R^2 (~0.035) but an extremely low RMSE (~0.020 μm). This outcome reflects the highly uniform NSA microstructure, which narrowed the property distributions and reduced variance across the dataset. Consequently, the model explained minimal variance but consistently predicted values that closely aligned with the actual Ra measurements.

This analysis demonstrates that the type of material and its structure have a significant influence on the accuracy of machinability predictions. In NSA, using ensemble methods like the stacking regressor proved more effective by combining multiple models to understand complex feature interactions better. When predicting "Ra" in NSA, the random forest technique delivered high accuracy with a low RMSE, indicating that it provided reliable estimates within a narrow property range, despite explaining only a small portion of the overall variance.

These findings suggest that the diverse structure of ITA facilitates the identification of patterns associated with machinability, which can be efficiently detected by tree-based models such as RF. Conversely, the more uniform structure of NSA necessitates the employment of more sophisticated techniques, such as ensemble models or neural networks, to uncover nuanced, treatment-specific patterns. Overall, these findings highlight the importance of selecting a predictive methodology tailored to the distinctive material properties to achieve more accurate predictions.

The ITA samples exhibited a wide range of properties, including strength, hardness, and toughness. These variations helped our random forest models identify meaningful patterns, particularly those related to the ease of machining the materials. On the other hand, the NSA samples generally showed more consistent characteristics, staying within a narrower range. This necessitated the development of more sophisticated models to uncover the subtle connections between different features.

For the ITA samples, XGBoost was somewhat helpful in predicting surface roughness (Ra). It did n't explain much of the variation, with an R^2 of around 0.098, but the predictions were close enough to be practically useful, with an RMSE of about 0.495 μm. When it came to predicting the machinability index, the random forest approach yielded the best results, achieving an R-squared value of approximately 0.201. It seemed to handle some of the more obvious non-linear patterns in the data, which makes sense considering the varied microstructure of the ITA samples—mostly pearlite–ferrite bands mixed with bainite and martensite regions. Such structural variability introduced wider spreads in toughness and strength values, providing patterns that random forest could successfully exploit.

This level of precision is highly valuable in industrial applications, where surface finish control is more critical than variance explanation. Conversely, the machinability index in NSA proved more challenging to predict. Experimentally, the stacking regressor did n't perform very well, with an R^2 close to zero (−0.002) and higher error measurements. This suggests that the model experienced difficulties in generating accurate predictions. A potential explanation is that the yield strength and impact

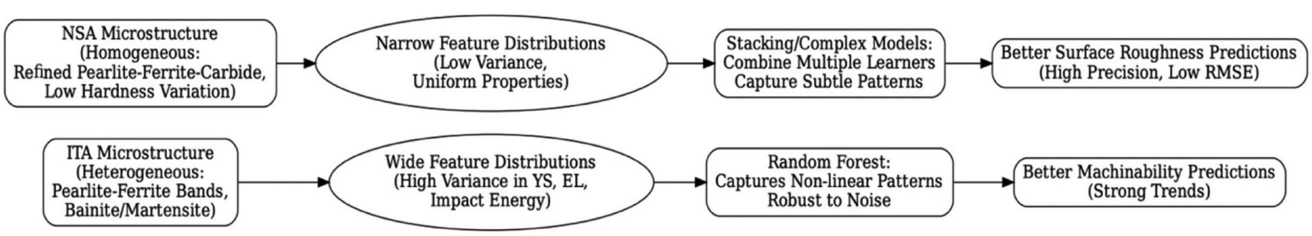

FIG. 3. Conceptual schematic linking heat treatment, feature distributions, machine learning model choice, and prediction performance. ITA produces a heterogeneous microstructure, leading to wide feature distributions that favor random forest models for machinability predictions. NSA produces a refined and uniform microstructure, resulting in narrow feature distributions that require more complex ensemble models (e.g., stacking regressor) for accurate machinability predictions, while random forest yields high-precision surface roughness predictions.

energy exhibited a minimal variation under NSA treatment, thereby complicating the model's ability to discern distinct patterns or trends.

The surface roughness for "ITA" samples yielded moderate results using XGBoost. The R^2 value was low (approximately 0.098), indicating a weak correlation; however, the RMSE was around 0.495 μm, which is acceptable for machining purposes. It means that the model was n't perfect, but it was still helpful. It has better input features, but it could still be improved. The machinability index for "ITA" samples showed that random forest performed best. It exhibited a clear upward trend and had the highest R-squared value (0.201) for all cases. This suggests that it captured key patterns in the data, especially for well-understood, regularly heat-treated samples, such as "ITA."

The surface roughness for "NSA" samples, as predicted by the random forest model, had a very low R^2 (0.035) but a relatively small RMSE (0.020 μm). This indicates that the predictions were very close to the real values, even though the model did n't explain much variance. It remains valuable for precise work where tight surface finish control is crucial. The "NSA" machinability index was the hardest to predict. The stacking model showed no discernible pattern ($R^2 = 0.002$). It struggled to learn from the current data, indicating a need for better or more detailed features, such as microstructure or phase types, or even utilizing more advanced models like neural networks.

Consistent with previous research, our findings confirm that no single model performs best across all tasks and materials.[34] Random forest has done well in the past with tool wear and surface finish, and here, it performed best for ITA machinability. On the other hand, NSA's unpredictability supports the idea that new materials need richer, more tailored data. Overall, this result shows that the right model depends on both the material and the prediction target. Even when R^2 is low, models with low RMSE can still be very useful.

Taken together, these results reveal that ITA's heterogeneous microstructure supports a stronger trend capture in machinability, while NSA's refined and uniform microstructure enhances prediction precision for *Ra*. The findings demonstrate the treatment-dependent nature of machinability prediction and underscore that, although low R^2 values are associated with high RMSE values, they still provide meaningful industrial insights. For instance, in surface finish-critical applications, NSA predictions are highly reliable despite the low variance explanation.

It should be noted that identical input parameters were employed for both ITA and NSA samples; the differences observed in model performance originate from the distinct feature distributions generated by the two heat treatments. In ITA samples, XGBoost yielded moderate results for Ra prediction, with a low R^2 (~0.098) but acceptable RMSE (~0.495 μm), suggesting that although the variance explanation was limited, the individual predictions remained close to the actual values. Regarding the ITA samples, the random forest performed quite well, with an R^2 of approximately 0.201, effectively capturing the complex, non-linear patterns caused by the diverse properties. For NSA samples, it predicted Ra very accurately, with an RMSE of approximately 0.020 μm, despite an R^2 of roughly 0.035, indicating limited variance due to the uniform microstructure, yet still yielding high prediction accuracy. Predicting the NSA machinability index proved more challenging, as the stacking regressor struggled with narrow feature ranges, which limited trend detection. These results reveal that low R^2 with low RMSE can still be industrially relevant, especially in surface finish control, and emphasize the treatment-dependent nature of machinability prediction.

B. Feature importance analysis

The feature importance plots highlight which mechanical properties most strongly influence the model predictions. The feature importance results in Fig. 4 show that impact energy is the most influential factor across prediction tasks, as well as surface roughness and machinability index, for both ITA and NSA samples. This aligns with earlier studies that emphasize toughness as a crucial property in machining processes. Tough materials can absorb shocks, reduce vibration, and resist crack formation during machining.[35,36] The result is more conclusive, as impact energy is a direct measure of material toughness. Impact energy depends on several microstructural features such as grain size, phase distribution, and the presence of carbides or inclusions. They play a key role in how well a material absorbs shock and resists damage during sudden loading in machining processes.[37]

For ITA samples, surface roughness is also shaped by % elongation and Young's modulus. This supports past findings that ductile and stiff materials help produce a smoother surface.[38] These features help in influencing chip formation, vibration, and energy transfer during machining. When it comes to ITA machinability, yield strength and % reduction in area also play important roles. These properties are critical for managing machining resistance and thermal effects on tool wear. Together, these properties reflect how the material balances strength and plasticity during machining.[21]

In NSA samples, despite the novel heat treatments, Young's modulus and impact energy again lead in predicting surface roughness. This suggests that stiffness and energy absorption play a key role in determining surface texture. In the case of machinability, this study offers a clearer, data-driven perspective on the factors that influence samples, with impact energy and yield strength being the strongest contributors. It shows that together, these properties play a big role in how the material deforms and responds during machining processes.

These patterns indicate that, even with new alloy designs, the core mechanical properties remain the most important. In comparison with earlier research, this study offers a clearer, data-driven perspective on the factors that influence machining outcomes. It highlights impact energy and yield strength as reliable indicators, helping guide more brilliant material design and machining strategies. In summary, higher-strength steels present increased machining challenges due to the requirement of greater force for machining and accelerated tool wear. Softer steels are better able to maintain their shape throughout the machining process. Specific properties, such as ductility and stiffness, play a crucial role in determining the formation of chips, the development of cracks, and the management of vibrations. These factors collectively influence the final surface quality and the material's manufacturability.

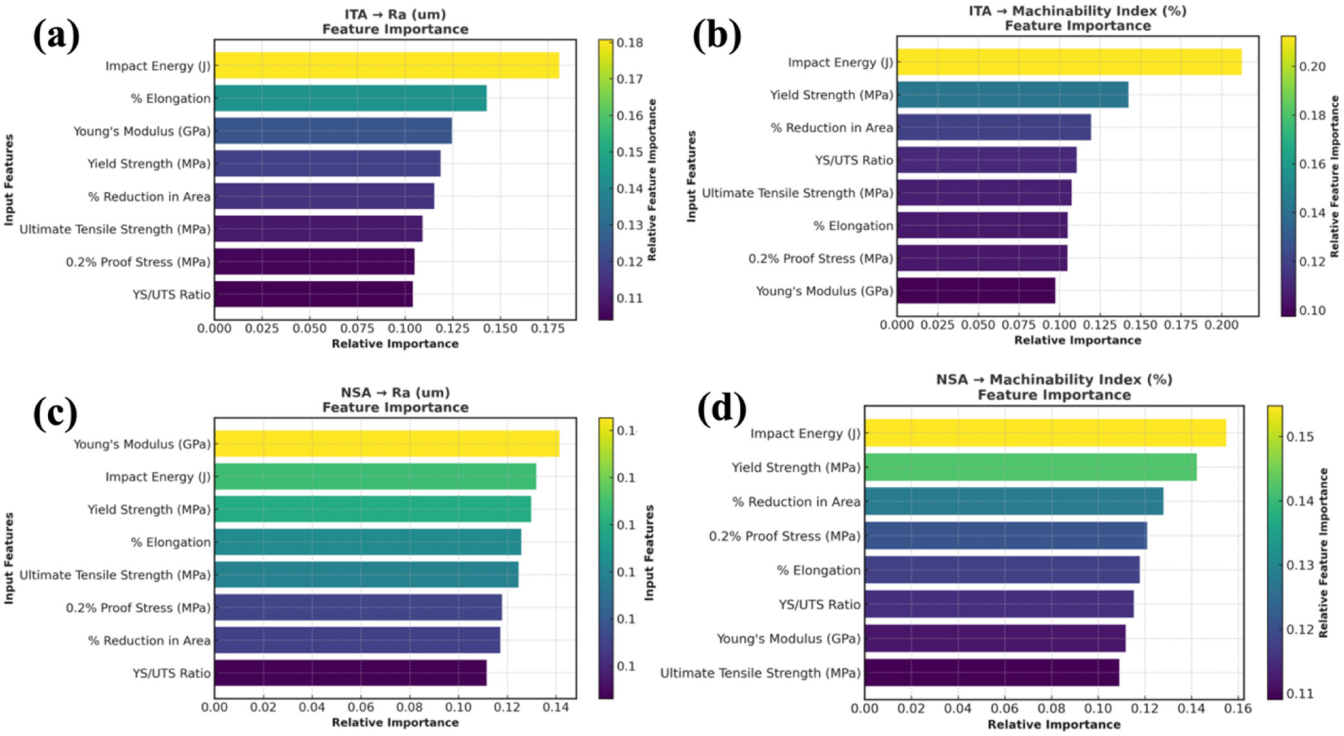

FIG. 4. Feature importance plots for predicting surface roughness (Ra) and machinability index (%) in Ni–Cr–Mo low-alloy steel subjected to two distinct heat treatments: conventional ITA and novel NSA. (a) For ITA Ra, the most significant characteristics are the impact energy, % elongation, and Young's modulus. This demonstrates how surface quality is affected by hardness, flexibility, and stiffness. (b) The ITA machinability index yields the highest ratings for yield strength and impact energy, indicating how these factors work together to create components that are stiffer and more difficult to machine. (c) For NSA Ra, the primary factors affecting surface finish projections are impact energy and Young's modulus. This makes logical sense because homogeneous microstructures require stiffness and resistance to vibration. (d) The impact energy and yield strength are again the most critical factors in the NSA machinability index. This means that toughness and strength are the best indicators of how easily a material can be machined. Impact energy was always the strongest feature in both treatments. This demonstrates the significance of stabilizing machining behavior to enhance the smoothness of machining performance.

C. Feature correlation heatmaps

The correlation heatmaps in Fig. 5 provide valuable insights into the relationships between mechanical properties and machining outcomes, including surface roughness (Ra) and machinability index (%), in both regular ITA and novel NSA samples. For ITA samples, surface roughness exhibits a weak to moderate correlation with % elongation and impact energy, while the machinability index shows a slight positive correlation with impact energy ($r \approx 0.27$) and a weak negative correlation with yield strength ($r \approx -0.14$). Interestingly, yield strength and UTS are slightly anticorrelated ($r \approx = -0.08$), indicating their independence in this alloy dataset, and they behave independently. In contrast, the NSA samples present a different picture: both Ra and machinability exhibit very low correlations with all input features. Only weak trends are visible; machinability shows a low positive correlation with impact energy ($r \approx 0.14$) and a slightly negative one with yield strength ($r \approx -0.05$). The remaining features also exhibit very little correlation with one another, indicating minimal overlap or redundancy in the data.

For standard heat-treated ITA samples, weak to moderate correlations were observed between surface roughness (Ra) and ductility or toughness (% elongation and impact energy). The machinability index exhibited a slight dependence on impact energy and yield strength. These trends are consistent with the feature importance analysis, reinforcing that strength and toughness are critical to machining behavior.

In novel heat-treated NSA samples, correlations were very weak across all features, reflecting the refined and uniform microstructure produced by the novel heat treatment, which narrows the spread of mechanical property distributions.

This shows that simple linear correlations are insufficient to describe machinability in novel heat-treated NSA samples. Instead, nonlinear machine learning models, such as random forest and XGBoost, are required to capture the combined influence of identifying hidden interactions among multiple features that simple pairwise correlation coefficients might overlook.

Thus, the correlation heatmaps serve as a diagnostic tool that helps us identify meaningful property-machining relationships in ITA while demonstrating why more advanced non-linear

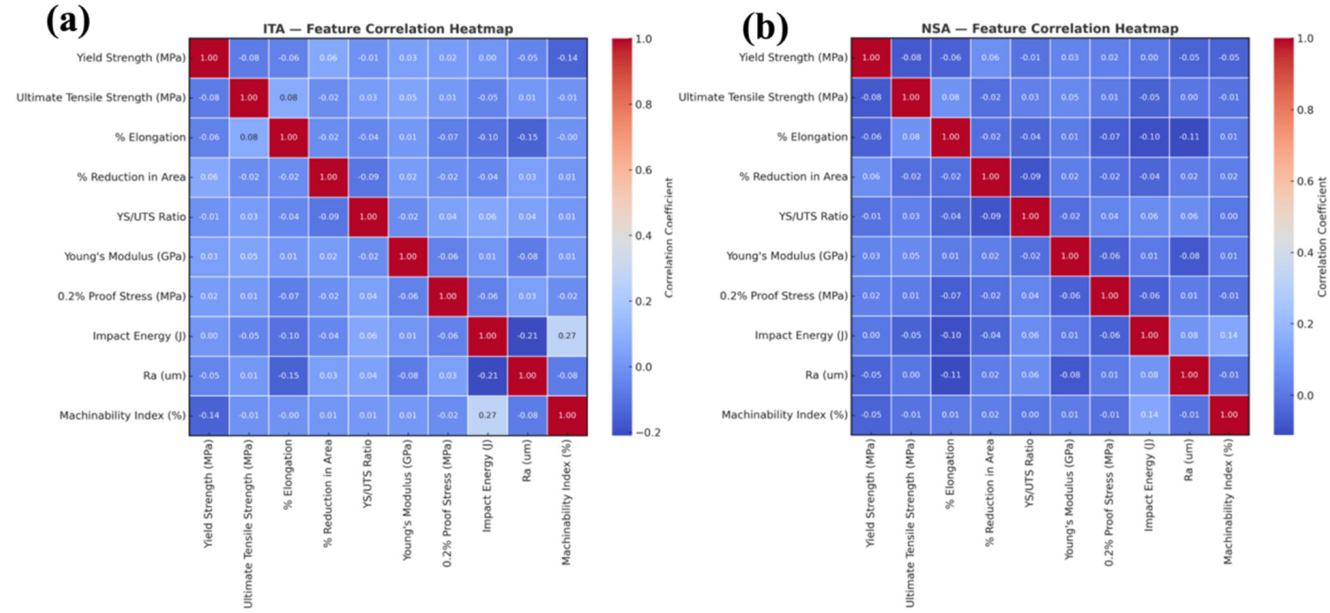

FIG. 5. Correlation heatmaps illustrating the relationships among mechanical characteristics, surface roughness (Ra), and machinability index (%) for (a) ITA and (b) NSA heat-treated Ni–Cr–Mo steels. In ITA samples, Ra has a weak to moderate relation with % elongation and impact energy, whereas the machinability index shows a modest positive correlation with impact energy and a weak negative correlation with yield strength. The patterns indicate that ductility and toughness affect surface finish, whereas toughness and strength impact machinability. In NSA samples, the majority of correlations are weak, indicating the homogeneous microstructure and confined property variability resulting from the novel heat treatment. The absence of strong linear trends highlights the limitations of correlation-based methodologies and validates the application of non-linear machine learning models, such as random forest and XGBoost, to identify hidden multi-feature interactions that are not evident in conventional pairwise correlations.

modeling approaches are necessary in novel heat-treated NSA samples.

These visualizations help determine whether any meaningful linear relationships exist between input features and machining targets. While a few moderate patterns emerged, especially in ITA samples, the overall results highlight the limitations of relying solely on linear correlations. Most relationships appear weak or non-linear, requiring the need for non-linear modeling approaches such as random forest and XGBoost. These algorithms are better at identifying hidden patterns and interactions that may not be apparent from surface-level correlations, which supports their use in the present study's predictive framework.

D. Prediction histogram comparison: Actual vs predicted

The histograms in Fig. 6 provide a practical view of how well the model captures the actual distribution of machining outcomes, including surface roughness (*Ra*) and machinability index, for both regular ITA and novel NSA samples.

The prediction of "Ra" in ITA samples aligns reasonably well with the central values of the actual distribution, but again, fails to reflect the range in the tails. This may be due to over-regularization or a slight bias in the model, possibly from smoothing during training. Importantly, for machinability in ITA samples, the predicted histogram tracks the central peak well but appears too smooth overall. This dampened shape suggests the model may be slightly conservative in its estimates, missing some of the natural variation seen in the actual data.

In NSA samples, the predicted values of "Ra" are tightly grouped around the mean, indicating that the model is precise. However, the narrower spread suggests that it may not fully reflect the variability present in the real data. In simple terms, it is hitting the center but not quite stretching to the edges. The predicted values of machinability in NSA samples match the peak of the actual distribution well, but the model underestimates both ends (tails) of the range. This indicates that while it is getting the average right, it is struggling to catch the extremes, something that could matter in edge cases during machining.

These plots are invaluable for understanding how well the model is trained and calibrated. They show whether predictions are too narrow, too flat, or missing high and low extremes. This feedback is essential when fine-tuning a model. It helps find the right balance between accuracy, generalization, and real-world applicability, particularly in machining, where minor prediction errors can have a significant impact on performance, cost, or tool wear.

E. Partial dependence plots

The partial dependence plots in Fig. 7 provide a clear illustration of how individual material properties shape the predicted machining outcomes, without the noise from other features. This

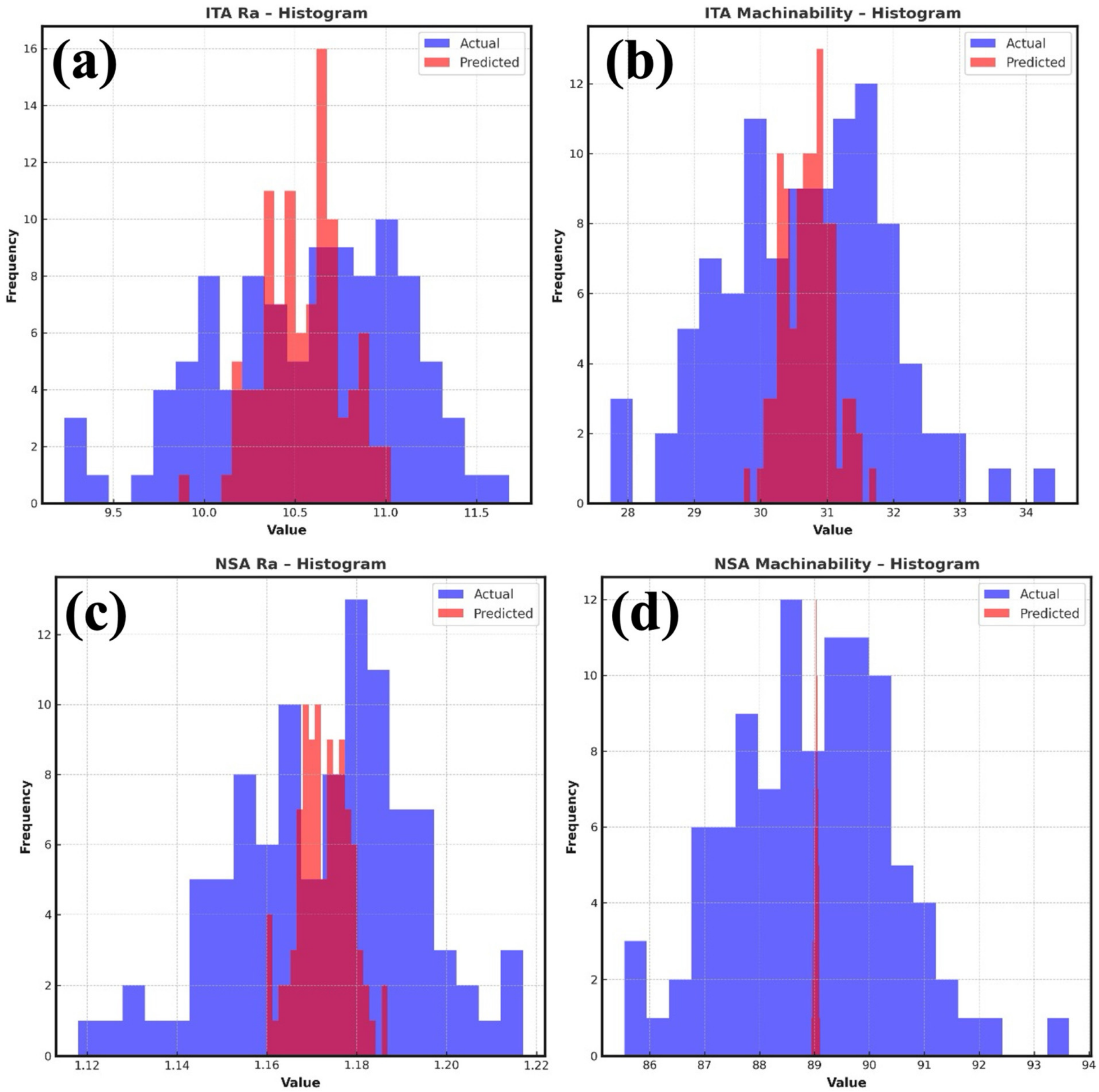

FIG. 6. Prediction histograms comparing actual and predicted distributions for surface roughness (Ra) and machinability index (%) across ITA and NSA alloys. Each subplot shows how closely the model's predicted values align with the actual values, offering insights into model performance, variance handling, and calibration across different targets and materials.

helps us understand how the model makes its predictions, and which material properties are having the biggest impact and in what way.

For ITA samples, the surface roughness (*Ra*), the left plot in Fig. 7(a) shows a clear trend, as impact energy increases, *Ra* decreases. In simpler terms, tougher materials lead to smoother surfaces.

This fits well with real-world applications, where materials that absorb energy well tend to resist chatter and tool vibration, giving a cleaner finish. On the right, in Fig. 7(a) % elongation has a more complex, non-linear effect. There is a drop in *Ra* with increasing ductility up to a point, but then the benefit levels off. This suggests there's an optimal range for elongation beyond which further gains do n't improve surface quality much.

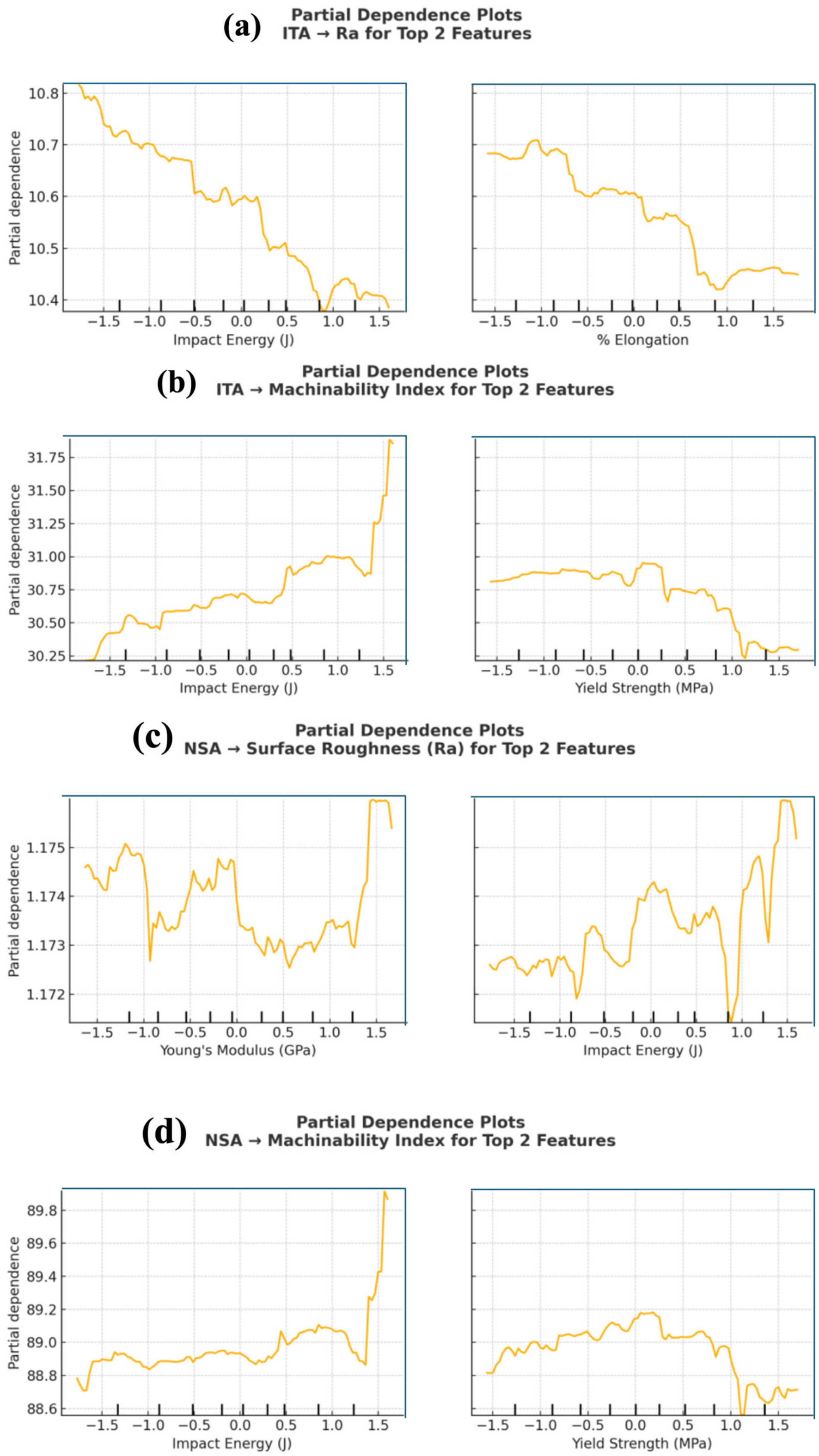

FIG. 7. (a) and (b) Partial dependence plots showing the effect of the top two most influential features on model predictions for surface roughness (*Ra*) and machinability index (%) in both heat-treated samples. (a–b) In ITA samples, *Ra* and machinability index influenced by impact energy, % elongation, and yield strength. The *x*-axis values in all the plots are normalized values and appear the same ranging from −1.5 to +1.5. (c) and (d) illustrate the "Ra" and machinability index in NSA samples, influenced by Young's modulus, impact energy, and yield strength. Each plot visualizes the marginal impact of a single feature on the predicted outcome while holding other variables constant.

In the case of the machinability index in ITA samples, impact energy again plays a key role, showing a steep rise in predicted machinability as toughness increases. This makes sense as materials that absorb energy without fracturing are easier to control during the machining process. Yield strength, however, exhibits a flattening or slightly declining trend, suggesting that beyond a certain strength level, further increases do not improve it and may even negatively impact machinability. This reflects what is often observed in industry, where robust materials are more challenging to machine and wear tools out faster.

In NSA samples, the patterns are generally weaker. For surface roughness, the influence of Young's modulus and impact energy is less pronounced but still present. The curves suggest that both properties affect *Ra* in a non-linear way, with possible zones where surface roughness is minimized. The pattern is uneven, suggesting that minor changes in properties can still influence machining behavior. Finally, for the machinability index in NSA samples, impact energy again shows a strong positive effect. Machinability increases rapidly as toughness rises, a similar trend observed in the ITA samples. Yield strength follows a weaker trend. It improves machinability up to a point and then levels off, showing diminishing returns beyond a certain threshold.

Across all these plots, impact energy is the most consistently influential property. It affects both surface roughness and machinability in both types of samples. Other features, such as % elongation, Young's modulus, and yield strength, also play a role, but their impact depends more on the specific material and machining target. These plots help highlight where each property has the most impact. That makes them especially useful for engineers who need to fine-tune alloy composition or machining conditions. With this kind of insight, it is easier to determine which properties to focus on and when further changes may no longer be beneficial.

F. Key features validation

Our findings indicate that impact energy (toughness) and yield strength are reliable indicators for guiding more effective material design and machining strategies, which, in turn, relate to machinability and surface finish. These results are consistent with previous research and studies on low-alloy steels. The relationship derived between Charpy impact energy and fracture toughness is widely used in prior studies.[39] Multiple studies have reported quantitative links between the Charpy impact test and fracture toughness, which serve as a controlling factor for stability and surface integrity during machining.[40] Tougher steels demonstrate greater resistance to chatter and crack initiation at the tool–workpiece interface, thereby enhancing surface roughness (Ra). This correlation is corroborated by turning studies on low-alloy steel, where vibration amplitude and cutting forces are indicative of surface finish quality.[41]

However, yield strength controls cutting resistance and tool loading; increasing yield strength generally raises cutting forces and heat, degrading machinability and surface finish if other factors are held constant. Recent studies have shown that as materials become harder and stronger, they also become more difficult to machine. Our feature rankings also reveal that yield strength is a crucial factor in predicting how easily a material can be machined.[42,43]

The machinability of low-alloy steels has been experimentally studied using various cooling methods and parameter settings. These studies consistently demonstrate that surface quality and tool wear are closely related to the steel's strength and toughness.[44]

Finally, previous machining studies on Ni–Cr–Mo and AISI 4340 steels confirm that toughness improves surface roughness, while strength governs the trends in machinability. It also emphasized that machinability decreases with increasing hardness and yield strength, which supports the present results. These consistencies validate the conclusion that impact energy and yield strength are reliable indicators for guiding machining strategies and alloy design.[45]

These findings are consistent with prior research concerning Ni–Cr–Mo and analogous steels. It has been demonstrated that increasing toughness can improve surface stability and reduce chatter, thereby producing a superior surface finish (Ra) during machining of AISI 4340 steels.[43]

Conversely, higher yield strength is typically associated with increased machining forces and accelerated tool wear, which can make machining more challenging, as evidenced by studies on AISI 4340 under both dry and wet conditions.[44] Additionally, reviews suggest that as hardness and strength increase, machinability typically becomes more challenging.[45] This perfectly corroborates the patterns we have identified with our machine learning models.

Many reviews highlight that tree-based and collaborative methods outperform linear regression when predicting machining outcomes involving complex property interactions.[5,34] Our results are in line with this, as random forest and collaborative regressors provided more accurate predictions than simple linear models.

All these points strengthen the conclusion that impact energy and yield strength are good indicators for predicting machinability and surface roughness. They also show that machine learning models are effective in capturing the effects of different treatments on machining behavior.

IV. CONCLUSIONS

This research integrated novel heat treatments with machine learning models to forecast the machining characteristics of Ni–Cr–Mo low-alloy steels. Two heat treatments were evaluated: conventional isothermal annealing (ITA) and a novel multi-step procedure (NSA). Mechanical parameters, including yield strength, impact energy, elongation, and stiffness, are used as input features to forecast surface roughness (Ra) and the machinability index. The NSA produced a uniform and refined microstructure with reduced hardness variability. This enhanced machining stability and facilitated the accurate prediction of Ra. ITA produced a diverse microstructure with greater variability in its characteristics. This enabled the detection of more distinct patterns in machinability. Impact energy and yield strength were identified as the most reliable indicators of machining outcomes. Impact energy signifies toughness, which influences vibration resistance and surface finish. Yield strength affects cutting resistance and tool wear, which directly influence machinability. These findings correspond with existing research on alloy steels, confirming that toughness and strength are essential indicators for machining. The models exhibited moderate R^2 values while attaining minimal prediction errors. This signifies that they offer dependable point forecasts notwithstanding constrained variance explanation. The NSA is suitable for situations where a consistent surface finish is essential. ITA plays a vital role in understanding machinability behavior and guiding the selection of machining parameters. This methodology reduces reliance on trial-and-error machining and promotes data-driven process planning. The present study demonstrates originality through the integration of a unique NSA heat treatment technique with predictive modeling. Future research should incorporate microstructural data and hybrid models to improve predictive accuracy. These advancements are expected to advance alloy design, machining optimization, and cost-effective manufacturing methods in high-performance steels. Despite modest statistical fits (R^2 values), the models achieved low error margins, which are of greater practical significance. In practice, NSA is recommended when stable surface roughness is critical, while ITA can be chosen when machining performance needs adjustment, providing the industry with a clear basis for selection. This paradigm minimizes reliance on trial-and-error machining. It integrates material characteristics, heat treatment design, and machining results into a unified predictive process. Future enhancements should utilize microstructural characteristics and hybrid models to augment predictive accuracy. These measures will enhance the precision of machining predictions and support data-informed process planning in high-performance steels.

SUPPLEMENTARY MATERIAL

Mechanical properties data for the regular "ITA" and noble "NSA" heat-treated samples are provided in the supplementary material.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Arun Kumar Behera: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Abhinav Anand:** Data curation (equal); Formal analysis (equal); Methodology (equal); Visualization (equal); Writing – review & editing (equal). **Ram Krishna:** Conceptualization (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Supervision (equal); Visualization (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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