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Reviewed Paper

A MACHINE LEARNING MODEL TO PREDICT MECHANICAL PROPERTY OF DIRECTED ENERGY DEPOSTION PROCESSED LOW ALLOY STEELS

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Abstract

Directed Energy Deposition (DED) was developed to manufacture high-performance steel components with intricate geometries. Nonetheless, identifying the complex relationships in alloy composition, cooling rate, thermal history, and mechanical properties remains a significant challenge. Machine learning (ML) algorithms are progressively equipped to address this challenge via interpretable, and data-driven modeling. In this work, an ML-driven model is introduced to predict high-accuracy tensile strength, yield stress, and hardness properties while offering insight into the underlying factors that drive mechanical performance. A dataset comprising 2430 analyses via JMatPro by varying low alloy steel compositions is used to train ML models. Multi-Variable Linear Regression (MVLR) and Polynomial Regression (PR) are then applied to extract critical insights from DED-processed steels. This paper demonstrates that the proposed ML algorithms enhance defect prediction accuracy of DED-processed low alloy steels, offering a valuable pathway to advance metal additive manufacturing.

Keywords: Directed Energy Deposition (DED), Machine Learning (ML), Multi-Variable Linear Regression (MVLR), Mechanical Properties Prediction, Ensemble Learning.

1 Introduction

Directed Energy Deposition (DED) is an innovative metal additive manufacturing (AM) technique that builds parts directly from 3D models by melting and depositing material typically in powder or wire form [1]. DED using a focused energy source like a laser or electron beam. DED capability encompasses not only the manufacture of new materials but also the repair and customization of existing parts, rendering it highly advantageous for companies that manage intricate, high-cost elements [2, 3]. The flexibility of DED in handling various material compositions and complex geometry leads to more interest across sectors like aerospace, biomedical, and automotive. Unlike the conventional methods that remove material to shape a part, DED adds material precisely where it's needed, also able to reduce waste and decrease production time [4–6]. Still, challenges remain when it comes to ensuring the quality, consistency, and mechanical reliability of DED-built components which makes ongoing research and method control essential for broader adoption.

In DED processes, defects such as the keyhole porosity and lack of fusion may alter the microstructure of the built parts [7]. These defects are attributed to process parameters such as beam power, scan speed, cooling rates, temperature and material properties such as material thermal conductivity [7]. Also, continuous thermal cycles can change the mechanical properties, which can lead to problems of unexpected microstructure. Hence, DED-manufactured products need to satisfy the rigorous requirements of mechanical properties, which include yield strength (YS), ultimate tensile strength (UTS), and hardness value (HV), which are essential for the reliability of produced components and operational purposes in industrial applications and scientific research [8, 9]. For that dependability, it is necessary to understand the best process parameter, which will optimize to get the best results in experimental application time. Because examining the mechanical properties through the DED process is expensive and time-consuming. Therefore, before getting the experimental work simulation, it is important to find out the best parameters. For instance, Yahdollahi et al. [10] reported the mechanical and microstructural properties of 316L stainless steel fabricated by direct laser deposition (DLD). Even though experimental practice and simulation cannot easily bring about accurate computational prediction of the relationships between chemical compositions, grain size, cooling rates, thermal history, mechanical properties, and final product quality [11, 12]. Furthermore, predicting mechanical properties via simulations is arduous and requires the amalgamation of numerous discrete and expensive simulations.

Given the constraints associated with acquiring extensive experimental or simulation datasets in DED, ML has emerged as a viable and cost-effective solution for predicting mechanical properties. In contrast to conventional experimental or simulation-based methods, ML models offer significant flexibility and scalability, enabling iterative refinement with minimal resource investment. JMatPro-generated simulation data which allows for systematic variation of alloy compositions, cooling rates, grain size, and thermal histories, ML models like MVLR and PR can be effectively trained to uncover complex, non-linear relationships between processing parameters and resulting properties such as YS, UTS, and HV [13, 14]. In DED systems, this hybrid technique not only improves prediction accuracy but also helps optimize processes. The application of ML in this domain still faces challenges mostly related to the essential variety of DED-generated materials and the restricted availability of high-fidelity training data, which remains modest compared to datasets usually used in more general ML domains.

Due to limitations in the availability of experimental data and the complexity of DED procedures, ML has increasingly gained much attention in DED for predicting the mechanical properties with limited simulation data from JMatPro and process parameters. In the past, ML has proved successful for DED in various applications. Xie et al. [15] applied wavelet transformation combined with CNNs to predict spatially dependent mechanical properties of laser-DED Inconel 718 and achieved an $R2$ value of 0.7. Carl et al. [16] also demonstrated the performance of Ridge regression, XGBoost, and a VGGNet CNN in predicting yield strength from a simulated microstructural dataset of DED-fabricated stainless steel 316L with an $R2$ of 0.84. In another study, Israt et al. [17] investigated the credibility of XGBoost for the prediction of tensile behavior of L-DED of SS 316, and the good performance, even with a lack of quality of data for input response, is noted. These works underscore the emerging significance of data-driven methods to describe the highly nonlinear relationships of DED process parameter metrics and mechanical behavior.

While some prior studies have already demonstrated the potential for machine learning for AM processes, such as a lack of experimental range, restrictive processing environments, and a focus on a single set of materials. To address these issues, this study presents a much larger and diverse data collection for predicting mechanical properties in DED processes. The result was an extensive data bank, comprising over 2430 simulation datasets, which are currently under development in terms of size. This extensive information enables the development of accurate and broadly applicable ML models for the prediction and optimization of key mechanical properties, including UTS, YS, and HV, between various DED parameters and low alloy steel systems. This work aims to address the pervading problem of data scarcity in AM research and establish a scalable, data-driven foundation for the DED process.

Based on these efforts, in this study, MVLR and PR models associated with ensemble learning approaches are tested to predict the key mechanical properties such as UTS, YS, and HV of DED printed low alloy steels. The presented approach is based on a JMatPro-induced dataset with sufficient chemical alloy compositions, cooling rates, grain size, and thermal histories to develop an interpretable, scalable, and cost-effective predictive tool for optimizing DED-manufactured components. This versatility enables the model to predict properties of materials not present in the dataset, including those recently developed. This comprehensive and flexible material represents a significant step forward in the field, as such a general framework had not previously been established.

2 Methodology

In **figure 1** provides an overview of the framework, including data collection mechanisms, dataset properties, used ML models, prediction goals, as well as model explanation. In this section, aspects of data collection, feature engineering, and the machine learning algorithm are demonstrated

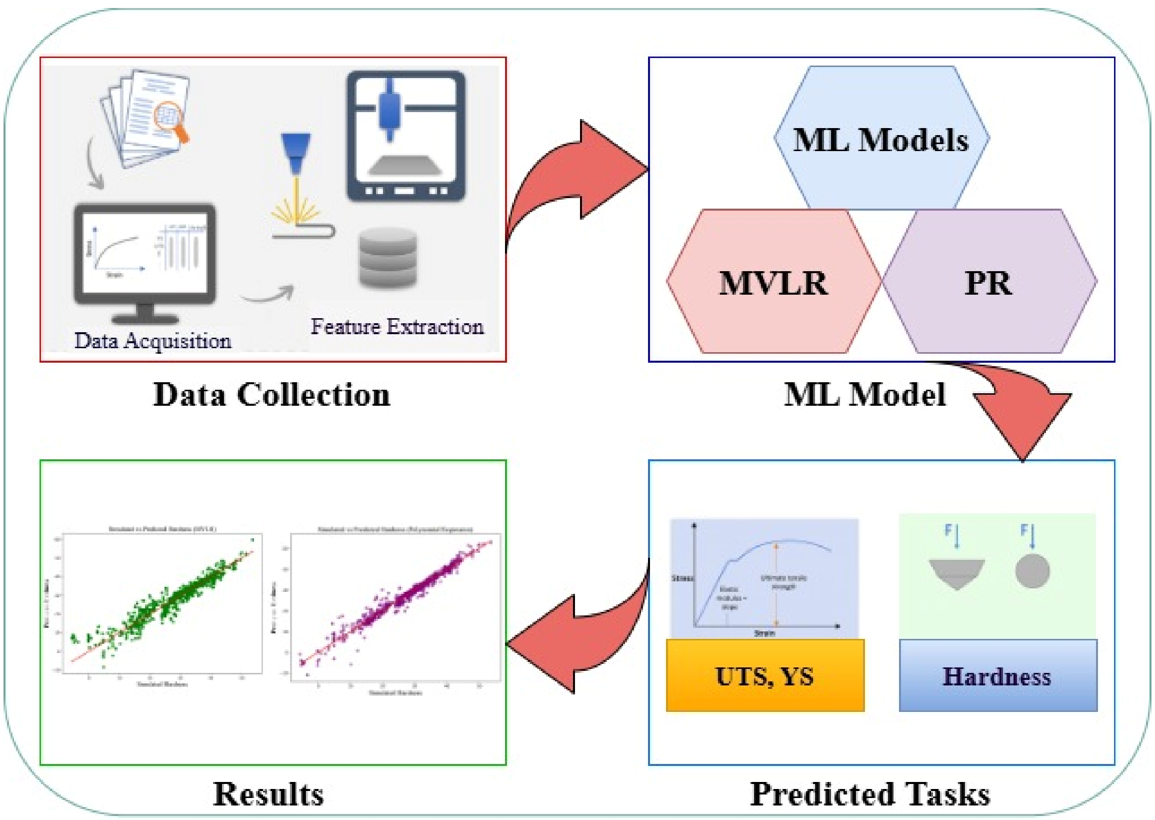

Figure 1: Workflow for Predicting Mechanical Properties Using Machine Learning Models in DED-Processed Alloys

2.1 Data Collection

The simulation and material composition data were obtained from JMatPro and the AM industries for their commercial machines. Data was extracted from figures and plots using an ML algorithm to ensure precision. Furthermore, the process parameters and materials properties were selected as input features for the ML models employed in this study.

2.2 Dataset

The benchmark dataset is generated from the JMatPro simulation, and it consists of 2430 datasets of DED processing conditions for low alloy steel material composition, thermal and cooling history, grain size, and the orientation employed for YS, UST, and HV. The input features are the input details and the properties such as YS, UTS, and HV. **Table 1** shows a statistical summary of different dataset labels, including their mean, median, and standard deviation. The descriptive statistics provided in this paper will highlight the spread and features of the data, thus providing an important insight into the general nature of the data. The compiled database incorporates a broad range of simulations performed with various materials, processing conditions, and post-processing approaches over a wide selection of DED processes. Subsequently, MVLR and PR ML models are applied to predict the mechanical performance of low alloy steel from the introduced input features performing different types of regressions.

Table 1: *Statistics of the dataset after data cleaning.*

	Variables	**Description**	**Min.**	**Max.**	**Mean**	**Median**	**SD**
Input Detector	C	Chemical composition (wt.%)	0.09	0.34	0.18	0.17	0.07
	Si		0.18	0.43	0.28	0.28	0.06
	Mn		0.43	1.44	0.66	0.6	0.258
	P		0.006	0.024	0.013	0.014	0.004
	S		0.003	0.022	0.01	0.009	0.003
	Ni		0.00	0.60	0.13	0.04	0.193
	Cr		0.00	1.12	0.44	0.11	0.458
	Mo		0.005	1.35	0.52	0.51	0.363
	Cu		0.00	0.25	0.08	0.07	0.061
	V		0.00	0.27	0.03	0	0.089
	Al		0.002	0.038	0.006	0.005	0.006
	N		0.0035	0.015	0.007	0.0078	0.002
	Grain Size		20.00	20.00	20.00	20	0.00
	Cooling Rate (C/s)	Cooling medium	Categorical	Furnace Cooling-0.01	Air Cooling-3.3	Ice Brine-375.00	
	Temperature		25.00	900.00	437.37	450	263.99
Output Properties	YS	Yield strength (MPa)	264.78	1557.14	732.71	727.24	244.80
	UTS	Ultimate Tensile strength (MPa)	371.63	1781.45	884.29	875.24	255.57
	HV	Hardness Value (HRC)	-5.61	53.65	28.44	29.49	10.81

2.3 Dataset Validation and Preprocessing

Dataset is applied by a structured validation workflow aligned with the MVLR and PR ML algorithms before training. First enforced schema and unit checks and screened values against metallurgical limits; statistical outliers were flagged by z-scores [18, 19],

$$z_i = \frac{x_i - \mu}{\sigma} \quad (\text{removed if } |z_i| > 3) \tag{1}$$

and the IQR rule and outliers are removed if [18, 20],

$$x \notin [Q_1 - 1.5 \times IQR,\ Q_3 + 1.5 \times IQR] \tag{2}$$

For retaining only those extremes justified by process physics. Missing entries (rare in simulation exports) were dropped, and exact duplicates were removed. To prevent leakage, preprocessing lived inside scikit-learn pipelines: continuous inputs were standardized as $\tilde{x} = (x - \mu)/\sigma$; categorical cooling media were one-hot encoded. For MVLR, we modeled targets $y \in \{\text{UTS,YS,HV}\}$ as [21],

$$\hat{y} = \beta_0 + \sum_{j=1}^{p} \beta_j x_j \quad (\text{fit by RSS minimization}) \tag{3}$$

For diagnosing multicollinearity via variance inflation factor (VIF) for each feature [18],

$$j: \text{VIF}j = \frac{1}{1 - R_j^2} VIFj \tag{4}$$

where R_j^2 is from regressing x_j on the remaining features. For PR, we captured nonlinearity by expanding features to degree 3 and fitting [22],

$$\hat{y} = \beta_0 + \sum_{j} \beta_j x_j + \sum_{j \le k} \beta_{jk} x_j x_k + \cdots \quad (\text{up to degree 3}) \tag{5}$$

These steps yield a clean, physically plausible, and statistically well-conditioned dataset for reliable MVLR and PR training and evaluation.

2.4 Featurization

During the training of ML models, a careful selection of the input features is necessary to make accurate predictions and generalize well. This paper summarizes the featurization baseline in Figure 2 (presented as a figure excerpt), characterizing important features that control the mechanical response of DED processed low alloy steels. These include, but are not limited to, primary DED processing variables, precise alloy chemistries, thermal history descriptors, estimated cooling rates, grain size features, and build directions, all of which are known to significantly impact mechanical behavior. To approximate the complex, non-linear dependencies relationship between these attributes and target output, MVLR and PR models are employed for accurate and reliable prediction of UTS, YS, and HV.

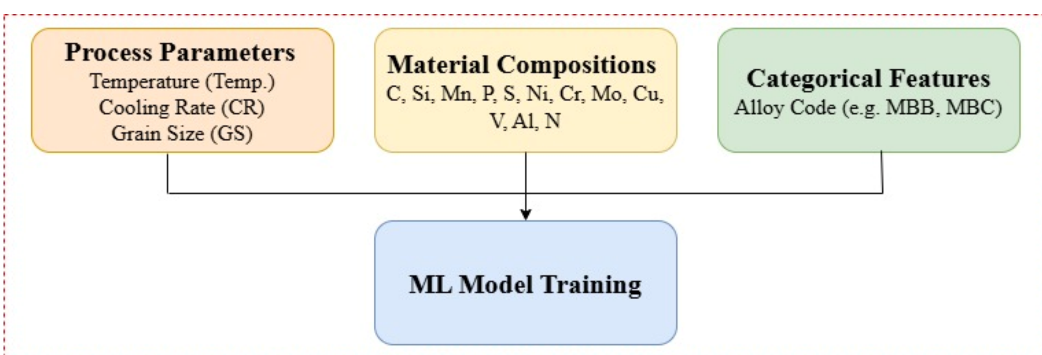

Figure 2: Featurization strategy used in this study for ML model training flowchart.

2.5 Models

The next part presents the predictive performance of the MVLR and PR ML models that were applied to the benchmark. This section is followed by a section that discusses further results.

2.4.1 Multivariate Linear Regression (MVLR)

MVLR is an important statistical technique for studying the linkage of a dependent single variable to several independent variables. MVLR serves as a simple and easy-to-use reference model for the prediction of mechanical properties of DED-processed low alloy steels [23]. The model assumes a linear relationship between the input features (chemistry composition, cooling rate, and process parameters) and target outputs (UTS, YS, and HV). The model estimates coefficients for each input variable that best fit the data by minimizing the difference between the observed and the predicted values (Residual sum of squares -R2). MVLR is formulated to solve the following equation in symbolic notations, in mathematical expressions shown in Eqn.6 [24]:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n \tag{6}$$

Where $\hat{y}$ is the predicted mechanical property, x_i is the input characteristics and β_i is the learned coefficient. One of the main advantages of MVLR is the high interpretability, which permits explicit quantification of the contribution of each processing or compositional variable to the mechanical response. This is particularly beneficial for understanding metallurgical trends in DED-produced steels. However, MVLR rests on some assumptions such as linearity, homoscedasticity, and no multicollinearity. To make good predictions, pre-processing includes feature engineering and correlation analysis. Despite its simplicity, MVLR is a method that provides interesting hints and serves as a robust benchmark to be compared with more complex models applied within this work.

2.4.2 Polynomial Regression (PR)

PR extends the concept of linear regression by including polynomial terms in the input features so that the model can detect non-linear correlations between the features and the output [25]. PR is employed in this work (Eqn.7) for the complex non-linear interrelations of DED process parameters, alloy compositions, UTS, YS, and hardness. The following equation describes the PR model [26]:

$$\hat{y} = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_n x^n \tag{7}$$

Here, $\hat{y}$ represents the predicted mechanical property, and x is the input variable(s), β_i are the coefficients obtained by training. This formulation allows PR to be capable of conforming not only to linear lines, but also to curves, thereby enhancing its capacity to model real material properties where the linear approximation is not sufficient.

One major strength of PR is its flexibility, as it can effectively model non-linear relationships in the data with low computational cost. In the context of DED processed steels, this is a great advantage to study the influence of subtle variations in thermal history and composition on mechanics [27]. However, increasing the degree of the polynomial increases the complexity of the model, which could lead to overfitting unless regularization techniques are applied [27]. To account for this in the model tuning, procedures of polynomial degree selection and validation were applied to ensure generalization and prevent high variability.

3 Results and Discussion

This section analyzed two regression models (MVLR and PR) for their predictive performance for the low alloy steel processed by the DED printer. The models were developed and optimized for three fundamental mechanical properties, namely, UTS, YS, and HV, based on a structured database implemented from thermophysical simulations and empirical process parameters. The precision of all models was evaluated with commonly used statistical parameters, such as R2, based on a series of performance diagrams through the MVLR and PR ML models. From the graphs, the data are non-linear, and polynomial regression performs better in determining critical mechanical properties. Thus, these results confirm the reliability of the chosen models and provide information about the intricate effects of DED process parameters on the mechanical properties of the parts produced. The predictive models utilized a comprehensive feature set, including elemental composition, process parameters (e.g., cooling rate, temperature, grain size), and a categorical alloy identifier (Alloy Code). The detailed performance of the models on each output parameter is discussed below. The predictive capabilities of ML models were employed on the benchmark dataset. Initially, the models were trained using baseline featurization, as detailed in **Figure 2**. These features were input into the ML models, and the results are shown in **Figures 3, 4, and 5** for both MVLR and PR models. In addition to cooling rates and thermal properties, the chemical composition of low alloy steel in terms of weight percentage (shown in **Table 1**) and elemental feature (**Figure 2**) was examined. These supplementary feature extraction techniques yielded improvements in prediction accuracy for applied ML models. **Table 2** shows the performance of the MVLP and PR algorithms below.

Table 2: *Summary of model performance for mechanical property prediction*

Category	MVLR (R^2)	PR (R^2)
Yield strength	0.78	0.86
Ultimate Tensile Strength	0.79	0.89
Hardness	0.81	0.90

As shown in **Figure 3**, the MVLR model **(Figure 3a**) captures the general trend in UTS but lacks sensitivity at the low and high strength ranges. It underestimates samples with fine grain sizes and large alloy additions (Cr and Ni) for low alloy steel [28]. The PR model (**Figure 3c**) describes well the curvature, with especially good agreement at the highest cooling rate, in the temperature effect and chemical composition strengthening regime. PR is also consistently in agreement with simulated results throughout the full UTS scale. The corresponding distribution of relative errors (**Figure 3d**) further demonstrates MVLR's limited accuracy, exhibiting a larger spread for the residuals as well as a few outliers (especially for the Ice-brine conditioned to high cooling rates). On the other hand, PR residuals are consistently low and centered, indicating a high stability to the highly changing chemical composition.

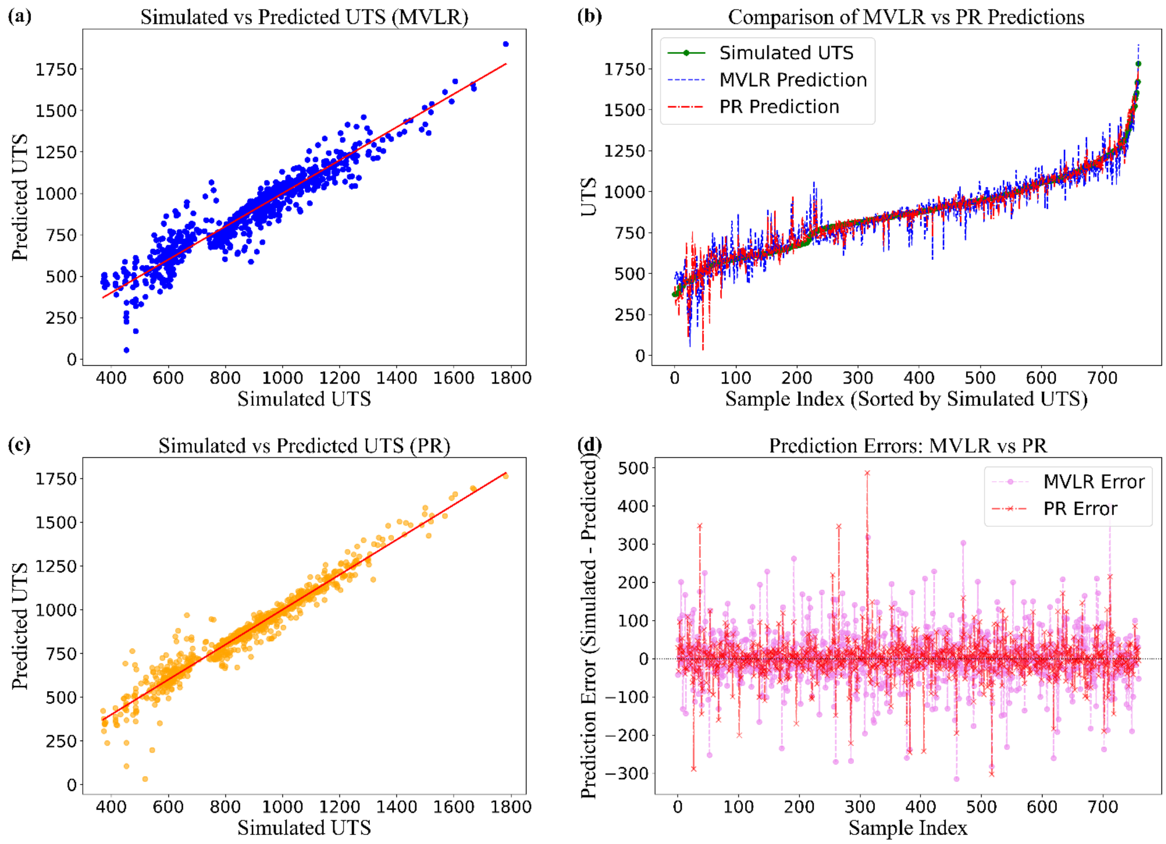

Figure 3: Performance of prediction UTS with the MVLR and PR ML models. **(a)** Simulated and predicted UTS by MVLR with a linear relationship, but some scatter at the lower and higher end of UTS. **(b)** Comparison between predicted UTS of MVLR and PR versus simulated UTS across the whole data set, in the nonlinear regime showing a better fit for PR approach. **(c)** simulated vs predicted UTS through PR with better fitting to the reference line compared to that by MVLR. **(d)** Error distribution of MVLR and PR, for which PR errors are more concentrated around zero with closer spread in both positive and negative side, representing better performance in UTS trends capturing accuracy and stability.

In **Figure 4** gives a clue to the YS prediction. MVLR (Figure 4a), meanwhile, produces a reasonable fit, but is not as good in mid-to-high YS ranges, which are related to steels with complex phase transformations [29]. As shown in Figure 4c, the PR model presents a tightly clustered band along the ideal, $y = mx + c$ line, indicating its better performance in capturing the complex non-linear relations between grain size, cooling rates, thermal history, composition, and process parameters as present in the DED-manufactured low-alloy steels. In terms of residual comparison (Figure 4d), MVLR yields considerably larger errors as YS increases, whereas PR generates lower residual errors for the dataset. These findings demonstrate the benefit of PR algorithm to capture the interaction between cooling rates, chemical composition, and process-dependent transformation paths.

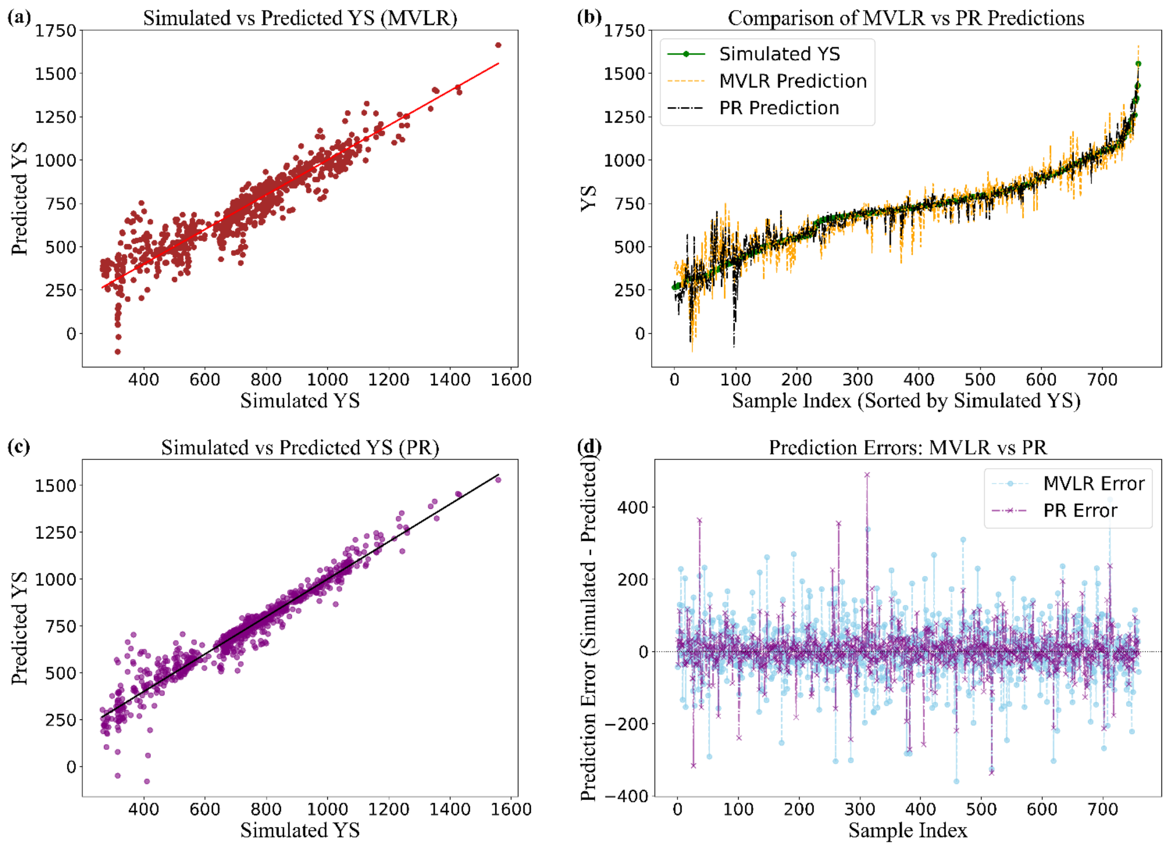

Figure 4: The prediction performance of YS models based on MVLR and PR algorithms. **(a)** Simulated YS vs. predicted YS by MVLR, a good linear correlation is observed along with larger scatter at higher YS. **(b)** YS simulated vs MVLR and PR predicted throughout the dataset; PR follows closest to the simulated curve, especially at mid to high YS level. **(c)** YS for simulated vs. predicated YS with PR, showing better fit to the reference line, compared to MVLR. **(d)** Error distribution of the MVLR and PR models, showing that PR gives a smaller and more evenly distributed residual, demonstrating its higher precision and robustness for YS prediction.

The results of the hardness value are displayed in **Figure 5**. The MVLR model (**Figure 5a**) exhibits a linear relationship; however, the predicted value begins to decrease in the increased hardness range due to the variation in cooling rate and carbon content, that has a large influence on the martensitic transformation [30]. The PR model (**Figure 5c**) is closely fitted to the ideal, $y = mx + c$ line, indicating that it can better depict linearity and non-linearity that arises from complex thermophysical interactions. The error plot (**Figure 5d**) confirms that MVLR possesses a higher variance, while PR residuals are additionally symmetric around zero. The superior stability and accuracy of PR in this case are consistent with its larger R^2 value (0.90 vs. 0.81), and it indicates the unique ability of PR to disentangle from data second-order interactions, such as grain size × composition and cooling rate × alloy class.

The comparison results of MVLR and PR predictions versus simulated values from low to high are shown in **Figure 3b**, **4b**, and **5b**. In all properties, MVLR appears to have a delayed and offset response at inflection points, which can be attributed to it not being able to capture the underlying nonlinear correlations between the input features. On the other side, PR captures the simulated trend lines better, hence differences are found especially in regimes with higher cooling rates as well as with rapid solidification, corroborating the need for higher order terms of DED data modeling.

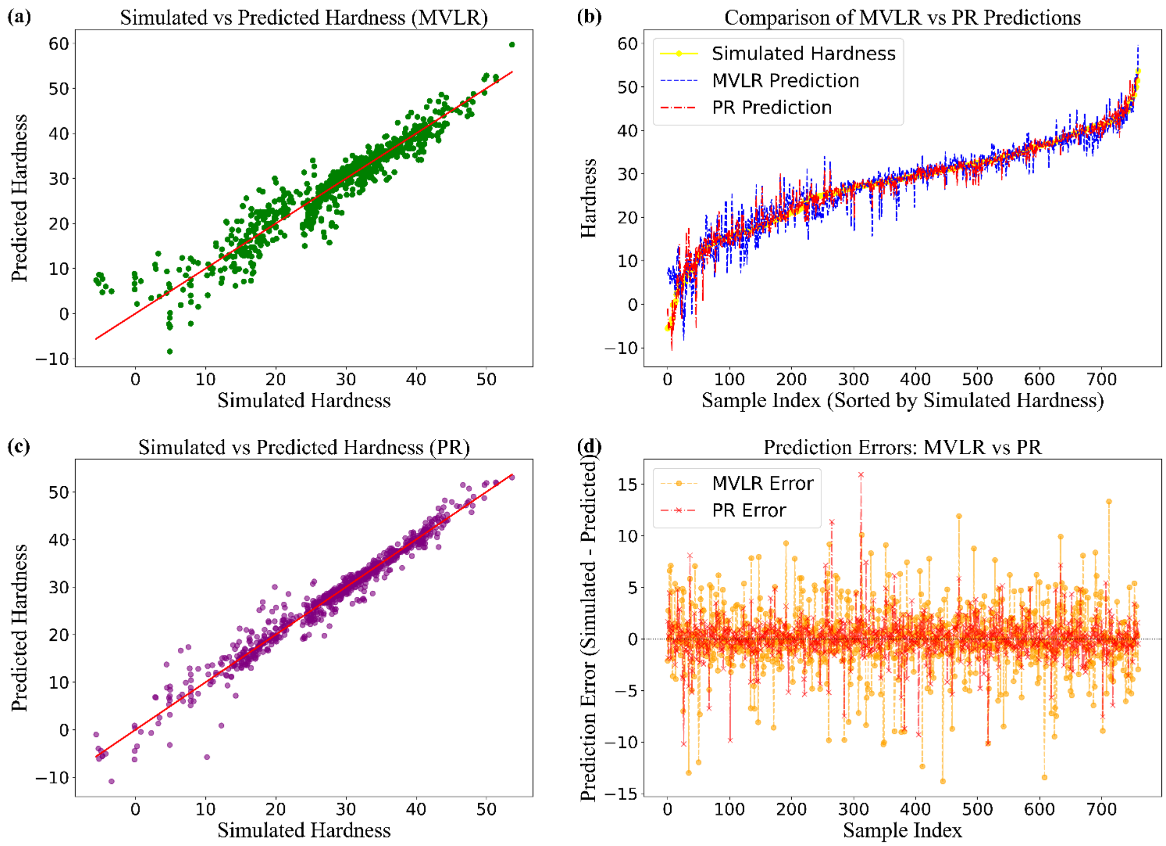

Figure 5: Prediction ability for hardness of MVLR and PR ML models. **(a)** Simulated versus predicted hardness by MVLR with overall good linearity, but a significant deviation at higher hardness levels. **(b)** Comparison of simulated hardness by MVLR and PR predictions over the dataset the comparison of PR vs MVLR predictions, across the dataset is shown. **(c)** simulated vs predicted hardness with PR presented in a good accordance with 1:1 line and smaller scatter than MVLR. **(d)** Distribution of the errors of MVLR and PR models, where PR errors are closer to zero, indicating that the errors of PR model are smaller and more symmetrically distributed.

Residual plots (**Figures 3d**, **4d**, **5d**) provide a clear distinction of model performance. Here, MVLR shows heteroscedasticity, with the residuals growing wider at higher property values, suggesting that prediction uncertainty increases with mechanical complexity. This tendency is more prominent in the specimens with segregation, grain boundary precipitation, or non-uniform solidification. Contrary to MVLR, PR shows heteroscedastic and normally distributed residuals, due to its improved power regulation of non-linear effects. These results also demonstrate PR's capability to accommodate physical behaviors and complex mechanisms, including thermal cycling effect, multi-phase coexistence, and synergistic alloying effects, hence a better and more reliable modeling platform in predicting DED properties. PR was more consistent across folds as the standard deviations were lower than those of MVLR. This behavior is evidence of PR's ability to represent complex process–microstructure, material class (via Alloy Code), and mechanical response relationships.

4 Conclusion

This study provides a comprehensive ML benchmark for predicting the mechanical properties of DED-processed low alloy steels. Among the mechanical properties, PR performed better than the MVLR model, implying that it is better at handling the non-linearity of interactions between the input variables. The performance difference is particularly high in hardness, with PR obtaining an $R^2 = 0.90$ against $R^2 = 0.81$ for MVLR. The PR also generated the higher R^2 values of 0.89 and 0.86, respectively, for UTS and YS compared to the MVLR of 0.79 and 0.78. Though not close to perfect correlation, these R^2 values demonstrate solid model fit for PR across the dataset, with MVLR performing well in the linear regions.

For this comprehensive simulation dataset encompassing various chemical composition DED processes of low alloy steel, specifically focuses on their effects on mechanical properties. MVLR and PR techniques were explored to enhance the performance of two ML models, while also examining evaluation metrics and hyperparameter optimization methods.

Beyond its predictive capability, the significance of this study is that it serves to encourage adoption by industry of DED. The present model gives a data-driven way for predicting UTS, YS, and hardness prior to processing, saving experimental costs, and promoting the qualifying of the alloy to the macroscale application. This enables faster material and process optimization including time, temperature and pressure as well as decreased trial and error in certification process for areas such as aerospace, automotive and power generation. Second, the system is scalable to large datasets and future machine learning algorithms, which allows the creation of industrial-strength user tools to be directly integrated into industrial DED manufacturing pipelines.

5 Future Work

Expanding on the current simulation-oriented scheme based on JMatPro-oriented featurization and regression-based modeling, the future work will focus on adding more simulation data to validate model predictions of UTS, YS, and hardness under realistic DED processes. To enhance the robustness of the models and to propagate the uncertainty, this work will extend to explore how the proposed framework incorporates a Physics-based DED-specific featurization that leverages "JMatPro" simulations to extract key input parameters such as material composition, grain size, cooling rate, and thermal properties relevant to mechanical behavior. Also, it integrates a suite of flexible ML algorithms along with customized evaluation metrics to form a robust foundation to predict mechanical properties. Furthermore, in this study MVLR and PR as interpretable models were also the baselines, more complicated ML approaches, such as Random Forests, XGBoost and Neural Networks, will also be attempted when the dataset is expanded. For enhancing interpretability, Explainable AI (XAI) techniques are employed to analyze feature importance and their influence on model prediction. Such algorithms have performed well within materials informatics and, when integrated with explainable AI, can trade off predictive accuracy against interpretability to offer scalable decision-support tools to industry for DED process. In parallel, explicit data-driven models will also be constructed using MVLR and PR to provide transparent and analytical insight into the mechanical property predictions of DED-processed low alloy steels.

Author Contributions: AR: Writing, review and editing, Writing original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data Collection, and Training. **MHA:** Writing, review, editing, Data Training, Supervision. **MAM:** Review and editing. **AWM:** Review and edit. **FL:** Writing, review and editing, supervision, Project administration, Funding acquisition.

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