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Article

# Advancing Automated Machining: Prediction of Surface Roughness in High Entropy Alloy Coatings Using a Novel Stacking Ensemble Machine Learning Model

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## Abstract

Digitalisation of mechanical engineering necessitates the use of predictive tools that are explainable and allow for more rapid analysis. The study began with cold spraying (CS) of high entropy alloy (HEA) coatings,  $Al_{0.1-0.5}CoCrCuFeNi$  and  $MnCoCrCuFeNi$  coatings at nitrogen gas temperatures of 650, 750, and 850 °C. The surface roughness,  $R_a$ , was measured using profilometry and microscopy techniques. The data set comprised 20 samples with varying experimental conditions and seven measured parameters (five input variables and surface roughness ( $R_a$ ) as the output. The stacking ensemble structure included three base learners, Linear Regression (LR), Extreme Gradient Boosting (XGBoost), and Gaussian Process Regression (GPR) with RidgeCV as the meta-learner. LR was chosen due to its simplicity and interpretability, GPR was chosen due to its ability to capture nonlinear trends with small datasets, and RidgeCV was used to stabilize the model by shrinking coefficients and reducing variance. This ensemble was compared with XGBoost, which is a powerful single machine learning approach. Results indicated that the stacking ensemble performed better than XGBoost in all the regression metrics. XGBoost reached 96.79% accuracy, RMSE of 0.22  $\mu m$ , MAPE of 3.32%, and  $R^2$  of 0.83, whereas the stacking ensemble achieved 97.26% accuracy, RMSE of 0.17  $\mu m$ , MAPE of 2.73%, and  $R^2$  of 0.89. The results validate that stacking ensembles can improve predictive and robust performance even in scenarios of small data. These novel stacking-ensemble and analysis methods can be broadened for future applicability.

**Keywords:** high entropy alloys; surface roughness; stacking ensemble; Linear Regression; Gaussian Process Regression; extreme gradient boosting; RidgeCV

## 1. Introduction

The advancement in metallurgical science has led to the creation of alloys with superior and more specific properties compared to individual metals. Traditionally, alloys primarily consist of one main element, restricting the compositional diversity and freedom. A revolutionary concept introduced by Yeh, known as High Entropy Alloy (HEA), diverges from this norm by incorporating a minimum of five primary elements, each making up 5-35% in atomic percentage [1,2].

Elements with smaller quantities, less than 5%, are said to be secondary alloying elements. Presently, current areas of interest include alloys of elements such as Al, Co, Cr, Cu, Fe, and Ni, and alloys of those based on these by other elements or substitutions [3]. The potential for discovering new alloys remains vast. HEAs are recognized for their structural and functional capabilities, owing to a high mixing entropy that encourages the formation of solid solutions with uncomplicated microstructures. The promising strength and hardness, enhanced stress and strain tolerance, and reduced temperature sensitivity of HEAs are due to multiple core effects, including high mixing entropy, lattice distortion, sluggish diffusion, and a cocktail effect [4,5]. HEAs' remarkable attributes and microstructural characteristics stem from several core effects, including high mixing entropy, lattice distortion, sluggish diffusion, and a cocktail effect [6]. Notably,  $\text{Al}_{0.5}\text{CoCrCuFeNi}$  alloy variants, through specific processing, have exhibited superior fatigue strength compared to many traditional alloys [7]. HEAs' tribological performance is influenced by their chemical composition; elements like Al, Fe, and Nb refine the grain structure and promote the formation of BCC phases, while Mn and Cr aid in developing hard phases [6]. C, N, B, and Si additions improve the creation of compounds or phase changes, causing the hardening and wear resistance to increase. The wear resistance of HEAs is greatly affected by the phase composition, where complex and ordered phases are better than traditional alloys having the same hardness [8]. Therefore, HEAs are currently undergoing growing use in creating very wear-resistant finishes using multiple deposition methods, with the addition of ceramic particles to the metal base to increase hardness and decrease wear rates [9–13].

One of the most significant parameters in any industrial application is the surface roughness, which can significantly affect the performance, life cycle, and aesthetic quality of any element that is produced [14,15]. The level of surface roughness affects not only the functional problems of the machining process, i.e., the friction, wear resistance, and fatigue lifetime, but also the very cost-effective performance of the production process in general [16–18]. As an example, the aerospace and automobile manufacturing industry needs the optimum surface roughness in order to determine the durability and reliability of the products to withstand the high-stress conditions [19]. Moreover, the accurate control of the surface roughness can potentially lead to an even better product performance and fewer demands of post-processing, which subsequently leads to more sustainable manufacturing processes [20]. This implies that the factors that the surface roughness is dependent on should be understood and well-controlled to ensure high-quality standards of industrial production [21].

Machine learning (ML) is a computational approach, the main goal of which is to identify systematic patterns in data sets that are not easily discernible by humans [22]. The use of extreme gradient boosting (XGBoost) in mechanical engineering has been successfully used in predicting process outcomes and material properties. Shahani et al [23]. developed an XGBoost model that predicts the static and dynamic young's modulus of intact sedimentary rocks based on inputs, including density, wave velocities, and uniaxial compressive strength. The model was more accurate than other ML and traditional regression methods and outperformed them. In a study by Mustapha et al [24]., XGBoost was used to predict the mechanical and physical properties of pervious concrete, including compressive strength, tensile strength, density, and porosity. The model achieved a high predictive accuracy, which shows robustness in the ability to deal with complex material behavior. Ou et al [25]. used the combination of XGBoost ensemble approaches and discrete element modelling to predict autogenous grinding mill throughput. The results of this provided a good agreement with the validation dataset. XGBoost showed high predictive performance with the test dataset. Gao et al [26]. proposed a distinctive material removal model with machine learning and acoustic sensing of robotic belt grinding of Inconel 718. Once training and optimisation have been carried out, the new k-fold XGBoost technique is introduced to the material removal (MR) model. The results of the test indicate that the values obtained via the model coincide with those measured. The model determined that the mean absolute percentage error (MAPE) of material removal was 4.37%.

Recently, the field of machine learning (ML) has proposed new methods of prediction. The stacking ensemble method is one of them. Baraheni et al [27]. used this technique in predicting

delamination and thrust in 72 carbon fiber reinforced polymers (CFRP) drilling runs. The superiority of the ensemble over the individual models was demonstrated by the fact that the MAE and RMSE values reduced substantially by up to 97%, 124% in the case of delamination, and 205%, 154% in the case of thrust force, as compared to the best base learner. Jones et al [28]. integrated the load-cell, accelerometer, and acoustic-emission signals into a three-level architecture and stacked a Random Forest (RF), an Artificial Neural Network (ANN), and XGBoost to forecast CNC-milling tool flank wear. The ensemble achieved an  $R^2$  value of 0.95 and an RMSE of 58.23. It was better than any single model and enabled prognostics and health management in real-time machining monitoring. According to Natarajan et al [29]., a two-stage pipelined structure with discretization of the output is proposed, where a regressor was controlled by a classifier. The resulting meta-model was more accurate, with the coefficient of determination ( $R^2$ ) of the XGBoost method more than 90% for all materials. This was significantly better than single-model models in predicting Ra.

This study used a novel stacking ensemble to predict the surface roughness of cold-sprayed HEA coatings from a limited dataset and compares its performance with a strong single ML model. The results indicated that the ensemble performs better in terms of accuracy metrics compared to the single model and can be used to make reliable predictions and parameter optimization using small data sets.

## 2. Materials and Methods

### 2.1. Experimental Setup

Data are required for any prediction method, including statistical or artificial ones. Data from 20 experimental conditions were collected [1]. The data set includes seven different parameters. Five of them are input measured before the setup experiment procedure, and one of them is surface roughness (Ra) as output (Table 1). High purities (>99.9%) of Al, (Mn), Co, Cr, Cu, Fe, and Ni elemental powders were processed through mechanical alloying (MA) to obtain octonary HEAs  $Al_{0.1-0.5}CoCrCuFeNi$  and  $MnCoCrCuFeNi$  (all in molar ratio). The designation of the samples was summarized in the following table. Based on these feedstocks, deposition of new HEA coatings on Mg substrates was performed by cold spraying at nitrogen gas temperatures of 650, 750, and 850 °C [30,31].

**Table 1.** The dataset used in this study [1].

Samples	Input Parameters				Output Parameters	
	Cut off (mm)	No. Cut off	Type	Temperature (°C)	Alloy type	Ra (μm)
1	0.25	5	Parallel	650	$Al_{0.1}$	5.81
2	0.25	5	Parallel	750	$Al_{0.1}$	4.48
3	0.25	5	Parallel	650	$Al_{0.2}$	4.36
4	0.25	5	Parallel	750	$Al_{0.2}$	5.85
5	0.25	5	Parallel	850	$Al_{0.2}$	5.09
6	0.25	5	Parallel	650	$Al_{0.5}$	6.35
7	0.25	5	Parallel	750	$Al_{0.5}$	5.73
8	0.25	5	Parallel	650	MN-HEA	5.58
9	0.25	5	Parallel	750	MN-HEA	5.55
10	0.25	5	Parallel	850	MN-HEA	5.78
11	0.25	5	Perpendicular	650	$Al_{0.1}$	6.01
12	0.25	5	Perpendicular	750	$Al_{0.1}$	5.20

13	0.25	5	Perpendicular	650	Al <sub>0.2</sub>	5.64
14	0.25	5	Perpendicular	750	Al <sub>0.2</sub>	5.87
15	0.25	5	Perpendicular	850	Al <sub>0.5</sub>	4.90
16	0.25	5	Perpendicular	650	Al <sub>0.5</sub>	6.62
17	0.25	5	Perpendicular	750	Al <sub>0.5</sub>	5.73
18	0.25	5	Perpendicular	650	MN-HEA	5.21
19	0.25	5	Perpendicular	750	MN-HEA	5.50
20	0.25	5	Perpendicular	850	MN-HEA	5.60

## 2.2. Data preprocessing

The most complex aspect of implementing a data set is describing qualitative factors alongside quantitative ones so that prediction algorithms can handle them. Therefore, categorical inputs must be encoded, called one-hot encoding. The surface roughness directions included two distinct categories (parallel and perpendicular); therefore, the qualitative variables were converted into a numerical format by the use of OneHotEncoding, similarly for alloy type. The parameters cut off and the number of cut off were not included in the analysis since these parameters were constant throughout the dataset. The Python code was run in Google Colab.

## 2.3. Accuracy metrics

Evaluating metrics is an important method to assess how well an ML regression analysis prediction model performs. Metrics are analytical and mathematical structures that are used to find how closely the projected output matches the actual result. Accuracy normalises the mean absolute error divided by the range of observed target values, as seen in equation (1). Some of the most commonly used metrics in research are mean absolute error (MAE) and root mean squared error (RMSE). According to equation (2), the RMSE measures the dispersion of the residuals and indicates how well the data fits the model. The lower the RMSE values, the better the models. Equation (3) shows that the MAE evaluates the precision of continuous variables independent of the direction of the mistake. Hence, the MAE is consistently less than the RMSE. The coefficient of determination ( $R^2$ ) represents the percentage of variation in the dependent variable that is elucidated by the independent variable using equation (4). It can range from  $-\infty$  to 1; the higher the values, the better [32]. A recent study [33] has shown that the coefficient of determination ( $R^2$ ) is more relevant than the other statistical criteria, such as RMSE and MAE, and that it is better to incorporate it with standard metrics to obtain more realistic judgments. The mean absolute percentage error (MAPE) is the most popular metric for predicting error, most likely because the variable's units are scaled to percentage units, making it simpler to interpret. This is calculated using equation (5) [34–36].

$$Accuracy = \left(1 - \frac{MAE}{Range\ of\ Actual\ Values}\right) \times 100 \quad (1)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{1}^n (Y_{pre} - Y_{act})^2} \quad (2)$$

$$MAE = \frac{1}{n} \sum_{1}^n |Y_{pre} - Y_{act}| \quad (3)$$

$$R^2 = 1 - \frac{\sum_1^n (Y_{pre} - \bar{Y}_{pre})^2}{\sum_1^n (Y_{act} - \bar{Y}_{act})^2} \quad (4)$$

$$MAPE = \frac{1}{n} \sum_1^n \left| \frac{Y_{act} - Y_{pre}}{Y_{act}} \right| \quad (5)$$

where  $Y_{act}$  is the actual value of the output results from the dataset,  $Y_{pre}$  is the predicted value from any machine learning algorithm,  $\bar{Y}_{act}$  is the mean value of the actual output, and  $\bar{Y}_{pre}$  is the mean value of the predicted output.

## 2.4. Machine Learning Implementation

### 2.4.1. Extreme gradient boosting

Extreme Gradient Boosting (XGBoost) is an effective algorithm that constructs a series of small decision trees, each at the current step correcting the previous errors. It copes well with missing values, regularizes complexity, and scales well on tabular data. With XGBoost, declared accuracy with tuning and early stopping is usually high, with much less overfitting and training time reduction [28,37,38]. In this paper, XGBoost was run using the xgboost library in Python. Figure 1 shows the structure of the XGBoost model employed in this study.

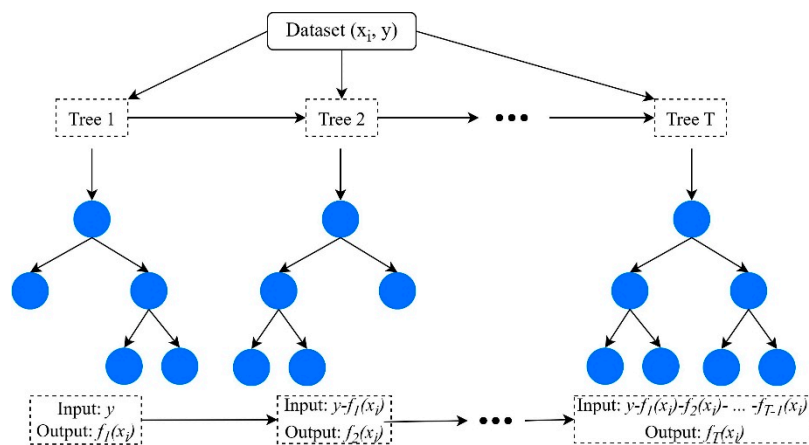


Figure 1. XGBoost model schematic diagram.

### 2.4.2. Stacking ensemble

A stacking ensemble approach was developed by averaging the outputs of different algorithms. This technique uses the predictions made by a number of base models to create a more accurate and reliable prediction. This model can be used in regression and classification problems. Several base models (ML models) are trained on the dataset in a stacking ensemble. A meta-model, a higher-level model, utilizes the predictions of the base models as inputs or training data. With the strengths of the base models, the meta-model can take advantage and make a final prediction [28].

The stacking ensemble architecture of this study is distinctive since it possesses three base-learner ML models and one ML meta-learner. The dataset was used to train the three base learners, and the Ra predictions were generated on a test set. The data used to train the meta-learner would be Ra predictions by the base-learners. The meta-model does not employ the original statistical features, but employs the base model predictions as features. The meta-model is validated against a test set as a way to give a fused forecast that is more accurate [28]. Figure 2 shows a diagram of the stacking ensemble architecture applied in this paper.

In this paper, a new stacking ensemble machine learning approach was employed. Linear Regression (LR) was chosen because of its ease of interpretation and simplicity, whereas Gaussian

Process Regression (GPR) was chosen because of its capability to capture complex nonlinear patterns in small data sets [39,40]. A cross-validated version of ridge regression, ridgeCV, was chosen as the meta-learner because it shrinks coefficients and decreases variance to stabilize the model and help avoid overfitting of combined base learners [41]. Therefore, LR, XGBoost, and GPR were used as the base learners, and RidgeCV was used as the meta-learner. This innovative stacking ensemble method, LR + XGBoost + GPR  $\rightarrow$  RidgeCV, has been selected because of the small size of the dataset, and allows avoiding overfitting and enhancing the predictive stability.

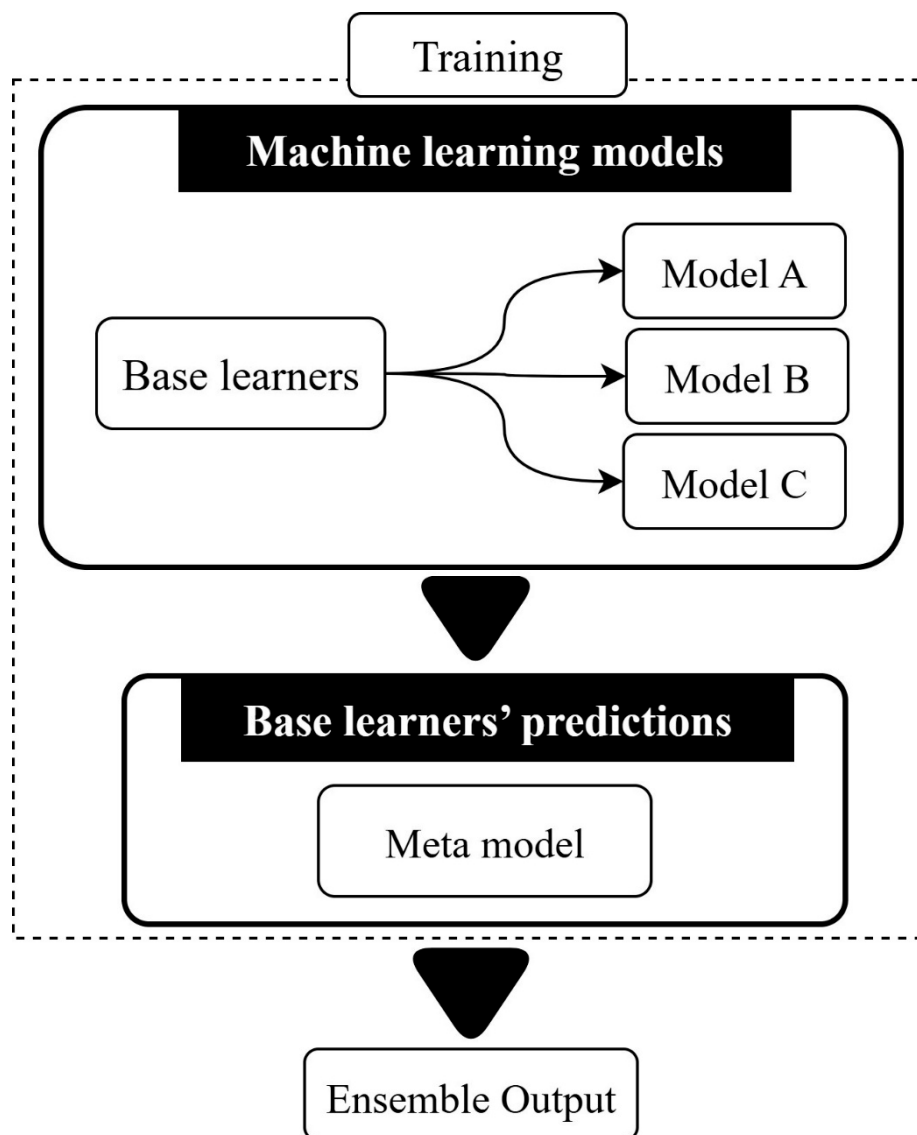


Figure 2. Stacking ensemble process flowchart.

### 3. Results and Conclusions

The analysis of variance (ANOVA) test has long been a vital mechanism for researchers performing studies on multiple experimental classes. However, it cannot provide precise information on differences among the various study groups or on complex combinations of groups. In order to measure the impact of input parameters on output ones, ANOVA is used to analyze all of the variability. Using this technique, we may divide the total variance into its component parts and give each part a degree of freedom in the model. In this work, three factors are taken into account as input controls, and the experimental value of this dataset was used to assess the surface roughness. For this data set, quadratic models were unable to display the important model analysis, as seen in Table 4, which displays the response surface. These models summarize the ANOVA of each response. Based

on the ANOVA in Table 2, the P-value of the Roughness type is 0.28, which shows that although this parameter plays a crucial role in the performance of the part among the other inputs, it is insignificant. A similar analysis was performed for other parameters, as shown in Table 2. It is clear that the Temperature is a more effective parameter than Alloy Type in this investigation. Overall, all parameters are not statistically significant at 95% confidence level ( $P > 0.05$ ) [42,43].

**Table 2.** The significance of each parameter.

Parameter	Sum sq	df	Mean sq	F	P-Value
Type	5.93	1	5.93	1.24	0.28 > 5%
Temperature	2.12	1	2.12	0.44	0.51 > 5%
Alloy type	15.53	3	5.17	1.08	0.38 > 5%
Error	66.92	14	4.78	-	-
Total	90.52	19	-	-	-

XGBoost, a widely used ML algorithm to make predictions on structured data, was used in this paper. According to the performance of the models, hyperparameters were selected in each base and meta-model. The hyperparameter tuning was performed by using Bayesian optimization via BayesSearchCV, a method in the scikit-optimize package. To make sure that the best parameter combinations were selected, cross-validation was applied to estimate the performance of each combination. The optimal hyperparameters for the XGBoost model are listed in Table 3. All hyperparameters of the stacking ensemble remained at default values, as implemented in scikit-learn.

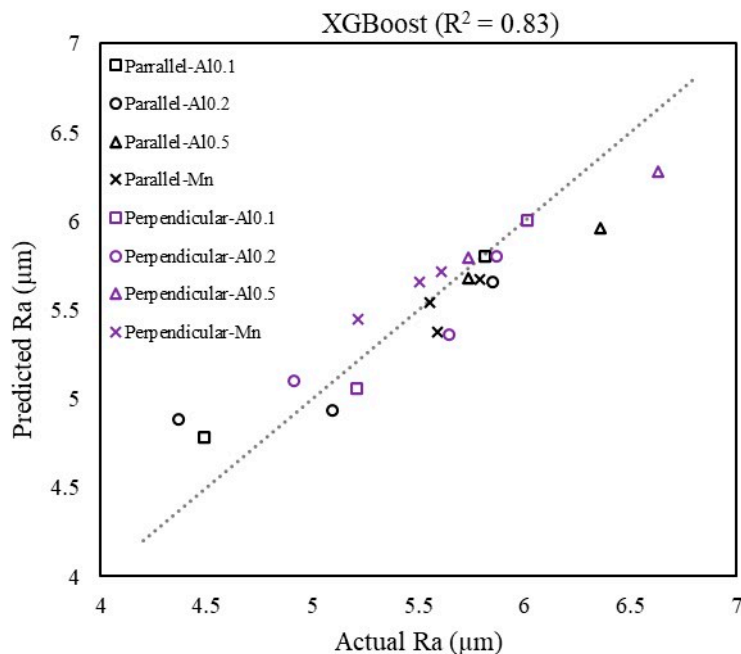
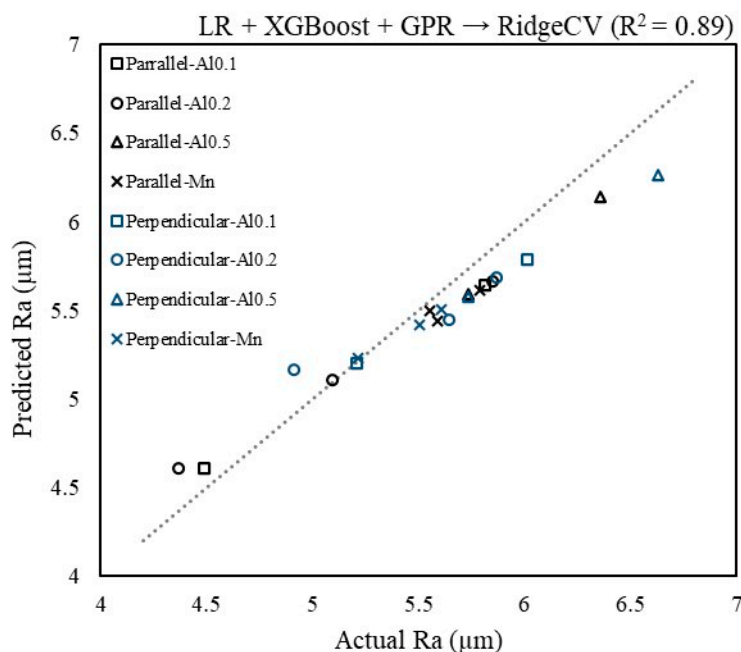
**Table 3.** Hyperparameters tuning for XGBoost.

Hyperparameter	Optimal value
Number of trees	400
Learning rate/tree	0.07
Maximum depth/tree	4
Subsample/tree	0.9
Column sample/tree	0.9
reg_lambda	5.0
reg_alpha	0.5

Accuracy metrics measure the proximity between predictions and actual values and allow fair comparison between models. The greater  $R^2$  and accuracy and smaller RMSE and MAPE prove that the model fits better and the residual variance is smaller, making predictions more reliable. On the evaluation set, the stacking ensemble performed better on all metrics compared to XGBoost. The performance of the two ML models in this study can be seen in Table 4. XGBoost resulted in approximately 97% accuracy, with an RMSE of 0.22  $\mu\text{m}$ , a MAPE of 3.32%, and an  $R^2$  of 0.83, whereas the stack produced 97.26% accuracy, an RMSE of 0.17  $\mu\text{m}$ , a MAPE of 2.73%, and an  $R^2$  of 0.89. This represents roughly a 23% reduction in RMSE and an 18% reduction in MAPE, with a 0.06 increase in  $R^2$ . Figure 3 shows each model's predicted surface roughness,  $R_a$ , values versus the actual ones for XGBoost and the stacking ensemble model with LR, XGBoost, and GPR as base learners and RidgeCV as the meta-learner (LR + XGBoost + GPR  $\rightarrow$  RidgeCV) is illustrated in Figure 4.

**Table 4.** Performance of the XGBoost and stacking ensemble models.

	Accuracy (%)	RMSE ( $\mu\text{m}$ )	MAPE (%)	R <sup>2</sup>
XGBoost	96.79	0.22	3.32	0.83
Stacking ensemble	97.26	0.17	2.73	0.89

**Figure 3.** XGBoost predicted vs. actual Ra values.**Figure 4.** LR + XGBoost + GPR → RidgeCV predicted vs. actual Ra values.

Based on the previous research, XGBoost is one of the most powerful algorithms; however, the stacking ensemble method enhances model robustness by using the power of various base learners. The ensemble methods, compared to single models, such as XGBoost, are that they can leverage the

strengths of various algorithms and address their weaknesses. In the present paper, where the small size of the data was an issue, ensemble methods proved especially useful, since limited data tends to overfit single models. Stacking ensemble is a broad and generally applicable framework [44,45]. The results of the current study verify that, with appropriate ML models, even in the case of limited data, it can provide more accurate and robust predictions when well-designed ML models (LR + XGBoost + GPR → RidgeCV) are combined.

#### 4. Conclusion

Modern manufacturing is based on data-driven approaches, but datasets are small and expensive to create, making prediction difficult. Machine learning has great potential, but in materials engineering, the models need to be accurate enough and interpretable to be useful in decision-making. Elemental powders of Al, Mn, Co, Cr, Cu, Fe, and Ni (>99.9% purity) were mixed through MA to produce HEAs  $Al_{0.1-0.5}CoCrCuFeNi$  and  $MnCoCrCuFeNi$ , which were deposited on Mg substrates by CS at temperatures of 650, 750, and 850 °C under Nitrogen gas conditions. Profilometry and microscopy methods were applied to measure the Ra, and thus the parameter set consisted of 20 experimental conditions with seven parameters: five input parameters and one output parameter, Ra. To overcome the problem of having little data, a stacking ensemble was created with LR, XGB, and GPR as base learners and RidgeCV as the meta-learner. All algorithms had complementary advantages. LR was interpretable, GPR was able to capture nonlinear interactions in small datasets, and RidgeCV stabilized the final model by shrinking coefficients and reducing the variance. The results of this ensemble were compared with the results of a powerful single ML model, XGB. The results indicated that the stacking ensemble performed better than XGB in all measures, attaining 97.26% accuracy, RMSE of 0.17, MAPE of 2.73, and  $R^2$  of 0.89, whereas XGB had 96.79% accuracy, RMSE of 0.22, MAPE of 3.32, and  $R^2$  of 0.83. These results support that stacking ensembles can improve predictive accuracy and robustness in data-limited settings and make them suitable for Ra prediction in CS HEA coatings and other applications in advanced material processing.

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