



# Machine learning for bead geometry prediction in 5083-H112 aluminum laser welding considering a challenging dataset

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## ABSTRACT

Laser welding of 5083-H112 aluminum alloy presents several challenges due to the material's high reflectivity and thermal conductivity. Consequently, it becomes difficult to establish a processing window that properly associates parameters with the desired weld bead geometry. This study aims to analyze and compare the predictive performance of five widely used machine learning regression techniques (Support Vector Regression, Decision Trees, Random Forest, K-Nearest Neighbors, and Artificial Neural Networks) for estimating weld bead geometry, considering a challenging dataset. It has small size, high process variance, and a discontinuity corresponding to the conduction-to-keyhole transition, thereby providing an important benchmark for assessing the models' capability of calibration on limited datasets. Weld bead width and penetration depth were selected as outputs, while scanning speed and power as inputs. A total of 99 bead-on-plate experiments were performed by combining 11 levels of laser power (1000 to 4600 W) and three levels of scanning speed (0.5, 1.0, and 4.0 m/min), within each parameter combination, process repeatability was accessed. The dataset was split into training (80%) and testing (20%) subsets. The best hyperparameters for each machine learning technique were determined by using GridSearch and five-fold cross-validation. The K-Nearest Neighbors technique resulted as the most recommended due to its low mean absolute percentage error, 4.68% for width and 8.35% for penetration depth, combined with the generation of smoother curves for physical plausibility. Feature importance analysis highlighted laser power as predominant factor. The proposed techniques demonstrate strong potential for industrial implementation, specially assisting technical personnel in defining process windows.

## 1. Introduction

Aluminum is a metal recognized for its mechanical strength combined with corrosion resistance and low density. These properties make it particularly attractive to the naval, automotive, and aerospace

industries. However, due to its physical characteristics, such as high thermal conductivity and the consequent rapid heat diffusion, it presents significant challenges for welding processes. Among the main issues are the occurrence of solidification cracks [1] and the formation of pores [2].

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Laser welding processes offer several advantages over tungsten inert gas (TIG) [3–5] and metal inert gas/metal active gas (MIG/MAG) [6,7], including, e.g. low distortion, narrow heat-affected zone, and high welding speeds [8–10]. However, it requires specific precautions, such as accurate sample alignment [11], and is strongly affected by the high reflectivity of aluminum, which limits the fraction of incident laser energy that is effectively absorbed [12]. Consequently, a thorough understanding of the underlying process, combined with reliable methods capable of identifying a suitable processing window, is essential to relate the parameters to the desired output variables properly.

One of the most important variables of the welding process is the weld bead geometry, specifically the width and penetration depth. According to Liang et al. [13], penetration is a fundamental requirement for welded structures. Ramiarison et al. [14] reported a correlation between the penetration-to-width ratio and ductility, recommending that this ratio remain as low as possible to enhance the mechanical performance of the joint. Shen et al. [15] highlighted that the selection of welding parameters is closely related to resulting bead geometry.

Traditionally, statistical methods such as Response Surface Methodology (RSM) have been employed to predict welding parameters. The idea of RSM is to establish a continuous variable surface model to evaluate factor interactions and to determine the relationship between the input factors and the response values [16]. This technique has been explored for predicting mechanical properties after welding [8,17], determining the distance for porosity mitigation, and assessing weld quality [14]. However, the RSM often fall short in capturing complex interactions [18]. Nonlinear relationships between welding parameters and the resulting characteristics are difficult to capture using polynomial fitting. Moreover, the high process variability further increases model uncertainty.

To address these limitations, machine learning (ML) techniques have emerged as powerful tools for modeling and optimization in welding processes. They are capable of learning from data (i.e., input–output relationships) without relying on an explicit mathematical/physical model. A key advantage of ML is its ability to predict highly complex nonlinear processes, and its application can optimize experimental designs by reducing material consumption and minimizing the number of trials [19]. Regression is one of the most established and frequently applied prediction techniques, offering a fundamental framework for quantifying relationships between input variables and target responses across a wide range of scientific and engineering problems [20]. Several ML techniques have been successfully applied in welding, including Support Vector Regression (SVR), Decision Trees (DT), Random Forest (RF), K-Nearest Neighbors (KNN), and Artificial Neural Networks (ANN).

Considering the SVR method, Barrionuevo, Mullo and Ramos-Grez [19] predicted the ultimate tensile strength (UTS) in joints of AISI 1045 steel and 2017-T4 aluminum alloy produced by rotary friction welding with laser assistance and achieved a better result compared to RSM. Liang et al. [13] improved the predictions of the backside bead (root) width from front side (face) signals. Asmael et al. [20] compared multiple ML techniques for predicting the properties after friction stir spot welding of AA7075-T651/Ti-6Al-4V alloys and found that SVR performed better.

Thankappan, Santhi and Vijayalakshmi [21], by using DT, estimated the clad bead geometry based on key MIG/MAG process variables. In this case, the SVR also performed well, and both methods outperformed traditional statistical models. Mothilal and Kumar [22] found the UTS of friction stir-welded (FSW) dissimilar AA7075 (Al–Zn) and AA5083 (Al–Mg) joints with an  $R^2$  score of 0.97.

Anandan and Manikandan selected RF to predict the peak temperature of the dissimilar AA7050-AA2014A FSW butt joint [18], and to predict the UTS for AA 2050, also in FSW joints [23]. Li et al. [24] found an  $R^2$  value of 0.93 on fatigue life prediction of spot-welded joints.

The KNN was applied by Thankappan, Santhi and Vijayalakshmi [21], Saha et al. [25] and Arif et al. [26] in welding applications, but did

not perform well when compared to other techniques.

Finally, ANN exhibited the highest performance in estimating the properties of aluminum FSW joints [26–29], fatigue life prediction of E36 steel welded joints [15], mechanical properties in TIG welding of preheated AISI 1045 steel [30], mechanical properties in cold metal transfer dissimilar stainless steels SS304L and SS439 joints [31], and resistance seam weld quality in secondary coated steels [32]. Additionally, physics-informed neural networks have demonstrated capabilities for 3D transient thermal simulation of MIG welding [33], showing the evolving landscape of computational modeling. Ventaka Rao et al. [34] observed that ANN predicted responses closer to experimental results compared to the physics-driven models for bead geometry in gas metal arc based additive manufacturing.

Considering the papers described above, it is evident that the choice of an appropriate ML technique must take into account the specific welding characteristics being estimated. The most suitable choice depends on the particularities of the available data, which in turn are influenced by the process, material, and welding parameters. Shen et al. [15] reported that, even when material and process were fixed, different ML approaches were more appropriate depending on the target output. ANN performed best for predicting bead height, SVR for width and cross-sectional area, and RF for contact angle.

Despite the increasing use of ML techniques in welding research, the current dataset presents unique challenges: it is relatively small, exhibits limited repeatability, and includes a discontinuity caused by the transition between conduction and keyhole regimes, an aspect not previously explored in the literature. Therefore, this study investigates and compares the predictive performance of five well-established ML regression techniques (SVR, DT, RF, KNN and ANN) in estimating weld bead width and penetration depth for this type of challenging data.

It is important to mention that ML techniques typically require a substantial number of experimental samples to ensure robustness and generalization capability. However, in the context of welding, conducting a large number of experiments entails significant financial costs, elevated energy consumption, and considerable environmental impacts, which conflict with the principles of sustainable manufacturing. As highlighted in Refs. [35,36], advancing sustainability in welding involves minimizing resource use, reducing waste generation, and improving energy efficiency throughout the process chain. Therefore, it becomes crucial to identify ML techniques that can deliver accurate and physically consistent predictions even when trained on limited datasets, balancing predictive performance with environmental responsibility and experimental feasibility.

The proposed models demonstrate significant potential for industrial implementation, particularly when coupled with real-time monitoring frameworks, robotic welding systems, or advanced process simulation tools. In addition, the study contributes to the ongoing transition toward smart manufacturing and Industry 4.0 paradigms, where automation, real-time adaptability, and minimal human intervention are key drivers.

## 2. Methodology

In this section, the procedure for data collection, the selected input and output variables, and the applied ML algorithms are presented. First, the experimental setup is described in detail. Next, the relationships between input and output variables are graphically illustrated, along with representative weld bead profiles. Finally, the ML techniques and their corresponding hyperparameters are outlined.

### 2.1. Data collection

In this study, plates with a thickness of 6 mm, a length of 120 mm, and a width of 75 mm were used in the experimental procedures. The base material was a 5083-H112 aluminum alloy, composed approximately of 4.5% magnesium, 0.15% chromium, and 0.7% manganese. The experiments were performed in the as-received condition, without

any specific surface preparation. The effect of the native oxide film on laser absorptivity was therefore not explicitly quantified, and the oxide layer thickness was not measured prior to welding. This choice was made in order to reflect realistic industrial welding conditions, in which surface condition and oxide thickness may vary. Possible influences of surface oxide on energy coupling efficiency and heat source stability are thus implicitly embedded in the experimental data.

The welding experiments were carried out using a fiber laser source manufactured by IPG Photonics®, model YLS 10000 (Ytterbium Laser System), with a wavelength of 1064 nm, a maximum nominal power of 10 kW, operating in continuous mode. This equipment was fitted with a laser welding head manufactured by Precitec®, model YW52, equipped with a collimating lens with a focal length of 150 mm and a focusing lens of 300 mm. In this optical configuration, the focal spot diameter of the laser beam was approximately 880  $\mu\text{m}$ , which was determined from the manufacturer's specifications and from standard Gaussian beam propagation calculations. It relates the spot diameter to the beam quality factor, laser wavelength, and lens combination. The optical setup was kept unchanged throughout all experiments to ensure full reproducibility. To protect the molten pool, argon shielding gas was supplied at a flow rate of 15 L/min, directed through a nozzle to the laser incidence point.

The motion was controlled by computer numerical control (CNC). All laser welding experiments were performed under a zero-defocus condition, i.e., with the focal plane positioned at the workpiece surface. The focal position was carefully set prior to welding and kept constant throughout the entire experimental campaign in order to ensure a stable and reproducible optical configuration. Combined with rigid clamping and CNC-controlled motion, this procedure ensured that defocus-related effects did not significantly influence molten pool morphology, weld geometry, or the experimental repeatability.

Considering the high thermal expansion coefficient of aluminum alloys, special care was taken to control thermal deformation during the experiments. All plates were rigidly clamped to the welding table in order to maintain stable boundary conditions and to minimize out-of-plane warpage during welding. This mechanical constraint ensured that thermal distortion effects did not significantly affect the laser-workpiece interaction conditions or the measurement of weld bead geometry. The clamping, together with the plate thickness (6 mm), provided sufficient stiffness to limit global deformation over the relatively short weld length employed in the experiments. No visible warping or misalignment affecting the laser-workpiece interaction or the focal position was observed during the welding trials. Consequently, welding-induced deformation is considered negligible with respect to the measured weld bead geometry and the stability of weld formation. Furthermore, all cross-sections used for bead width and penetration measurements were extracted from the central region of the welds, away from start and end transients, to ensure representative and undisturbed geometry evaluation.

The samples were prepared in accordance with the procedures specified in ASTM E3-11 to ensure consistent metallographic analysis. The specimens were ground using silicon carbide (SiC) abrasive papers with grit sizes of 80, 220, 400, 600, and 1200 mesh, with the grinding direction alternating by 90° at each step. After grinding, polishing was carried out using an alumina ( $\text{Al}_2\text{O}_3$ ) suspension with an average particle size of 0.3  $\mu\text{m}$ . Subsequently, the samples were chemically etched by immersion in Keller's reagent (2 mL HF + 3 mL HCl + 5 mL  $\text{HNO}_3$  + 190 mL  $\text{H}_2\text{O}$ ) for 30 s, in order to reveal the weld bead geometry and enable macroscopic analysis. The specimens were then examined under an optical microscope (OLYMPUS, model BX60 M) at 50  $\times$  magnification.

### 2.1.1. Inputs and outputs

Weld morphology was quantitatively assessed by measuring weld bead width and penetration depth from metallographic cross-sections, which were extracted from the central region of each weld. This

region corresponds to a steady-state welding condition and avoids start and end transients. The measured bead width and penetration depth values were then used as the target output variables for statistical analysis and machine learning model calibration. Fig. 1 illustrates a classical weld bead geometry, emphasizing the two primary dimensional features, width and penetration depth, that characterize the cross-sectional profile.

Table 1 presents the dataset used for technique development, listing the sample input and output variables considered in this study, specifically, scanning speed and laser power as inputs, and weld bead width and penetration depth as outputs. The welding thermal cycle was not directly measured. The process was parameterized using the nominal laser power and scanning speed, which are the primary controllable variables in industrial laser welding systems. While these parameters do not explicitly account for secondary effects such as variations in absorptivity, plasma or plume dynamics, and transient heat losses, the purpose of this work is to establish data-driven relationships between practical process settings and resulting weld bead geometry.

For each welding condition, three independent welds were produced, as identified by the sample IDs (e.g., A1–A3), resulting in a total of 99 samples for model training and validation. The scanning speed was tested at three different levels, i.e. 0.5, 1.0, and 4.0 m/min, whereas the power was varied at eleven levels, which are given by 1000, 2000, 3000, 3200, 3400, 3600, 3800, 4000, 4200, 4400, and 4600 W.

Fig. 2 presents the experimental results obtained for the weld bead geometry. Plot (a) shows the relationship between laser power and weld bead width, while plot (b) illustrates the relationship between laser power and penetration depth for three different scanning speeds. The plots reveal key characteristics of the dataset. First, the dataset is limited in size, which constrains the statistical robustness of training. In addition, it can be observed that some trials, particularly those at a scanning speed of 0.5 m/min, exhibited low repeatability, likely due to process instability under these conditions. Finally, a clear discontinuity is observed, corresponding to the transition from conduction mode to keyhole mode. These three characteristics represent potential challenges that may affect the performance and generalization capability of certain ML techniques.

Since welding experiments were carried out under CNC-controlled motion, it ensures stable and repeatable travel speed and welding trajectory throughout the entire experimental campaign. No noticeable deviations in the welding path were observed. Molten pool stability was primarily evaluated indirectly through the visual consistency of the resulting weld beads and through the repeatability of the measured bead geometry (width and penetration depth). While some geometric scatter was observed for specific parameter combinations, particularly near the conduction-to-keyhole transition, this variability is attributed to intrinsic process fluctuations rather than to trajectory deviations or motion control issues.

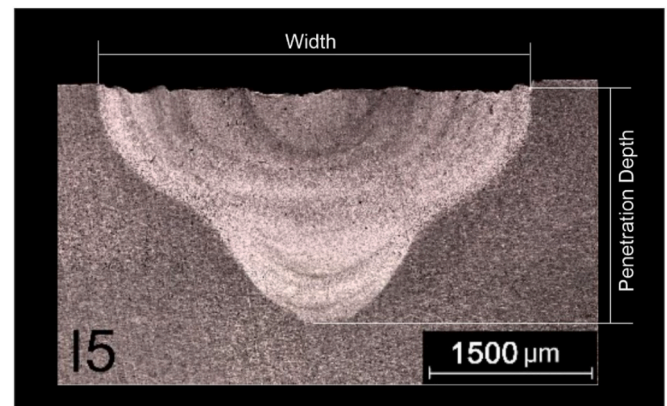


Fig. 1. Weld bead width and penetration depth dimensions.

**Table 1**

Laser welding test results on 5083-H112 aluminum alloy showing inputs (scanning speed and power) and the corresponding outputs (width and penetration depth) for all tests are presented.

| ID         | Inputs                 |           | Outputs           |                        |
|------------|------------------------|-----------|-------------------|------------------------|
|            | Scanning Speed (m/min) | Power (W) | Width (mm)        | Penetration Depth (mm) |
| A1, A2, A3 | 0.5                    | 1000      | 1.39; 1.50; 1.46  | 0.49; 0.50; 0.52       |
| B1, B2, B3 | 0.5                    | 2000      | 1.71; 1.76; 1.81  | 0.60; 0.59; 0.66       |
| C1, C2, C3 | 0.5                    | 3000      | 2.30; 2.46; 2.59  | 0.84; 0.90; 0.92       |
| D1, D2, D3 | 0.5                    | 3200      | 2.56; 2.78; 2.76  | 1.00; 1.06; 1.03       |
| E1, E2, E3 | 0.5                    | 3400      | 4.11; 3.65; 3.30  | 2.17; 1.37; 1.19       |
| F1, F2, F3 | 0.5                    | 3600      | 4.18; 3.74; 4.27  | 2.43; 1.48; 2.22       |
| G1, G2, G3 | 0.5                    | 3800      | 4.93; 5.27; 4.43  | 2.75; 2.70; 2.05       |
| H1, H2, H3 | 0.5                    | 4000      | 4.48; 5.11; 4.55  | 2.35; 2.97; 2.26       |
| I1, I2, I3 | 0.5                    | 4200      | 6.26; 6.30; 5.86  | 3.70; 3.28; 3.00       |
| J1, J2, J3 | 0.5                    | 4400      | 8.06; 7.27; 7.76  | 4.22; 4.10; 3.91       |
| K1, K2, K3 | 0.5                    | 4600      | 9.90; 10.01; 9.19 | 5.49; 5.92; 4.40       |
| A4, A5, A6 | 1.0                    | 1000      | 1.26; 1.47; 1.49  | 0.45; 0.50; 0.51       |
| B4, B5, B6 | 1.0                    | 2000      | 1.41; 1.83; 1.85  | 0.50; 0.62; 0.64       |
| C4, C5, C6 | 1.0                    | 3000      | 2.04; 2.40; 2.44  | 0.70; 0.76; 0.75       |
| D4, D5, D6 | 1.0                    | 3200      | 2.57; 2.51; 2.56  | 0.85; 0.85; 0.82       |
| E4, E5, E6 | 1.0                    | 3400      | 2.81; 2.83; 2.80  | 0.92; 0.95; 0.87       |
| F4, F5, F6 | 1.0                    | 3600      | 3.02; 3.06; 2.95  | 0.99; 0.96; 1.00       |
| G4, G5, G6 | 1.0                    | 3800      | 3.20; 3.18; 3.15  | 1.08; 1.12; 1.06       |
| H4, H5, H6 | 1.0                    | 4000      | 3.04; 3.70; 3.30  | 1.06; 1.67; 1.38       |
| I4, I5, I6 | 1.0                    | 4200      | 4.04; 4.02; 3.98  | 2.24; 2.23; 2.12       |
| J4, J5, J6 | 1.0                    | 4400      | 4.68; 4.98; 5.15  | 2.62; 3.02; 2.84       |
| K4, K5, K6 | 1.0                    | 4600      | 5.32; 5.41; 5.07  | 3.16; 3.01; 2.90       |
| A7, A8, A9 | 4.0                    | 1000      | 1.21; 1.29; 1.27  | 0.39; 0.40; 0.38       |
| B7, B8, B9 | 4.0                    | 2000      | 1.32; 1.58; 1.56  | 0.44; 0.50; 0.49       |
| C7, C8, C9 | 4.0                    | 3000      | 1.68; 1.86; 1.83  | 0.51; 0.54; 0.55       |
| D7, D8, D9 | 4.0                    | 3200      | 1.96; 2.00; 2.00  | 0.58; 0.58; 0.57       |
| E7, E8, E9 | 4.0                    | 3400      | 2.08; 2.09; 2.07  | 0.59; 0.57; 0.59       |
| F7, F8, F9 | 4.0                    | 3600      | 2.17; 2.17; 2.15  | 0.61; 0.59; 0.59       |
| G7, G8, G9 | 4.0                    | 3800      | 2.26; 2.26; 2.22  | 0.63; 0.66; 0.62       |
| H7, H8, H9 | 4.0                    | 4000      | 2.38; 2.28; 2.34  | 0.65; 0.62; 0.63       |
| I7, I8, I9 | 4.0                    | 4200      | 2.91; 2.80; 3.00  | 2.45; 2.06; 2.09       |
| J7, J8, J9 | 4.0                    | 4400      | 2.95; 2.94; 3.16  | 2.43; 2.30; 2.62       |
| K7, K8, K9 | 4.0                    | 4600      | 3.19; 3.04; 3.05  | 2.48; 2.63; 2.38       |

In the conduction mode, the laser beam is absorbed only at the surface of the workpiece. The absorbed energy, converted into heat, is then conducted into the bulk of the material, leading to the formation of a weld pool. This pool typically exhibits hemispherical geometry with shallow penetration, offering high stability. In contrast, under the keyhole mode, intense vaporization of the material takes place, and a cavity resembling a keyhole is generated due to the vapor recoil pressure acting on the molten metal. The laser energy is almost completely absorbed inside the keyhole. Compared with conduction welding, keyhole welding produces a deep-penetration weld characterized by its narrow and elongated profile [37].

Fig. 3 shows the macrographs corresponding to each welding condition, illustrating the geometric characteristics of the samples. It can be observed that the weld beads produced at 1000 W exhibit a typical conduction-mode profile, whereas those obtained at 4600 W correspond to the keyhole mode, regardless of scanning speed. The difference lies in the intermediate weld beads, where a discontinuity (jump in penetration depth) occurs. According to the literature, conduction mode generally occurs within the power density range of  $10^4$ – $10^6$  W/cm<sup>2</sup>, while the keyhole mode is observed above  $10^6$  W/cm<sup>2</sup> [38]. However, Fig. 3 demonstrates the influence of scanning speed on the occurrence of keyholes. It can be seen that the discontinuity separating the conduction and keyhole regimes occurs between 3200 and 3400 W ( $0.6 \times 10^6$  W/cm<sup>2</sup>) at 0.5 m/min, and between 4000 and 4200 W ( $0.7 \times 10^6$  W/cm<sup>2</sup>) at 1.0 and 4.0 m/min.

Another important aspect to be considered is porosity. In conduction mode, pores tend to be smaller and spherical, whereas in keyhole mode they are larger and exhibit irregular shapes. Hydrogen is generally recognized as one of the main factors responsible for porosity formation in fusion welding, especially in aluminum. The average temperature of a laser weld pool is significantly higher than that of arc welding, which leads to a much greater amount of dissolved hydrogen in the molten pool. In the case of keyhole welding, the cavity formed within the liquid metal is inherently unstable, and this instability further promotes the development of pores or cavities in the weld metal [39]. The formation of keyholes and pores during laser welding directly influences the weld bead geometry, introducing additional complexity to the training of the ML techniques.

## 2.2. Machine learning techniques

In this article, five ML regression techniques are evaluated for predicting the bead width and penetration depth resulting from laser welding of 5083-H112 aluminum alloy, based on scanning speed and power, namely: SVR, DT, RF, KNN and ANN.

The SVR technique seeks to determine a function that approximates the target variable while remaining within a specified tolerance margin ( $\epsilon$ ). Errors that fall within this  $\epsilon$ -insensitive region are disregarded, and penalties are applied only to deviations beyond this margin, thereby increasing the robustness of the model. The regression function is defined solely by the data points located outside the  $\epsilon$  margin (referred to as support vectors) which directly influence the shape of the regression line or curve. By employing kernel functions such as linear, polynomial, or radial basis function, SVR can capture both linear and nonlinear relationships, making it suitable for modeling complex behaviors. Its performance, however, is highly dependent on the proper selection of hyperparameters, particularly the penalty parameter C and the kernel parameter  $\gamma$  [25].

The DT technique estimates continuous outcomes by partitioning the dataset into smaller subsets. It builds a tree-like structure in which each branch corresponds to the values of input features. Internal nodes serve as decision points, whereas terminal leaves provide the final predictions. At each stage, the model selects the most informative feature to optimize the partitioning [29]. The main hyperparameters include maximum tree depth, minimum number of samples required to split an internal node, minimum number of samples per leaf, number of features considered at

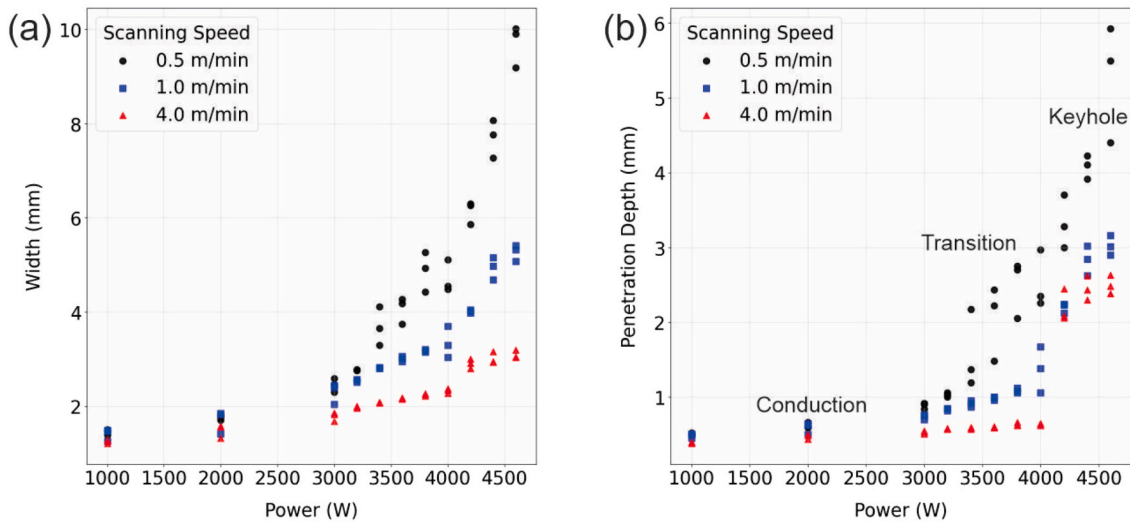


Fig. 2. Plots of weld bead width (a) and penetration depth (b) as a function of laser power and scanning speed.

each split, the function used to evaluate split quality, and the strategy adopted for selecting the split at each node.

The RF technique consists of multiple decision trees that operate collectively as an ensemble. The outputs of the individual trees are averaged to produce the final prediction, improving overall accuracy. This ensemble strategy reduces the risk of overfitting, which is often associated with single decision trees [25]. The hyperparameters are the same as those of DT, with the addition of bootstrap and the number of trees in the ensemble.

The KNN technique estimates the target value of a test sample by averaging the targets of the  $k$ -nearest training instances, determined by their distance in the feature space. It is characterized by its simplicity and effectiveness when applied to medium-sized datasets in regression tasks [21]. Its main hyperparameters are the number of neighbors considered for predicting a point distance metric, the weights (how each neighbor contributes to the prediction), and the parameter of the Minkowski distance metric.

ANNs are a class of computational models inspired by the biological brain. They consist of multiple layers of interconnected units that process input data and learn to identify patterns during training. An ANN is typically composed of an input layer, one or more hidden layers, and an output layer. During training, the network adjusts its connection weights based on the prediction error, typically by means of backpropagation [25]. The strength of this approach lies in its robust capability to model nonlinear behavior, enabling it to capture intricate and complex relationships [15]. Herein, the ANN tunnable hyperparameters are the number of neurons in the first hidden layer, number of neurons in the second hidden layer, dropout rate applied during training, L2 regularization factor applied to the weights, optimizer learning rate, batch size, and number of epochs.

The present study intentionally addresses a small-sample learning regime, comprising 99 experimental data points, which is representative of many laser welding studies where experimental campaigns are costly and time-consuming. Model robustness and generalization capability under limited data availability were assessed using five-fold cross-validation combined with GridSearch-based hyperparameter optimization for all investigated algorithms. In addition, model performance was evaluated on an independent test set (20%) using multiple metrics ( $R^2$ , MSE, and MAPE). Table 2 presents the values of the hyperparameters used for each algorithm. The codes were implemented in Python 3.12, and the main libraries employed were NumPy, Pandas, TensorFlow, Scikit-learn, Scikeras, and Matplotlib.

The feature importance was assessed using the permutation method [40], which consists of measuring the variation in model performance

when the values of a specific variable are randomly shuffled, thereby breaking its relationship with the response. This procedure enables the quantification of the individual contribution of each variable, since shuffling a relevant variable results in a significant reduction in the performance metric (in this study, the coefficient of determination  $R^2$ ). The method provides an interpretable layer of explainable artificial intelligence by quantifying how much each input variable contributes to the predictive performance of a model. This approach enables a clearer understanding of cause–effect relationships between process parameters and predicted outcomes. The process is repeated multiple times to mitigate the effects of randomness, and the mean values are reported. In this work, 30 permutations were applied.

Owing to the limited dataset size and the relatively low complexity of the employed algorithms, the computational cost of the proposed models is very low. Model training was performed offline and required negligible computational time on a standard CPU-based workstation, while model inference is effectively instantaneous. This makes the proposed approach suitable for practical use in offline process window definition and for potential integration into engineering decision-support tools.

The coefficient of determination ( $R^2$ ), mean squared error (MSE) and mean absolute percentage error (MAPE) are obtained from Equations (1)–(3), respectively.

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (1)$$

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (2)$$

$$MAPE = \frac{1}{n} \sum_{i=1}^n \frac{|y_i - \hat{y}_i|}{y_i} \times 100 \quad (3)$$

Where  $y_i$  are the actual values,  $\hat{y}_i$  predicted values,  $\bar{y}$  mean of the actual values, and  $n$  number of data points.

### 3. Results and discussion

This section presents the quantitative performance of the trained techniques and provides a detailed discussion that connects these empirical results to the core principles of ML theory and the complex physics of the laser-material interaction.

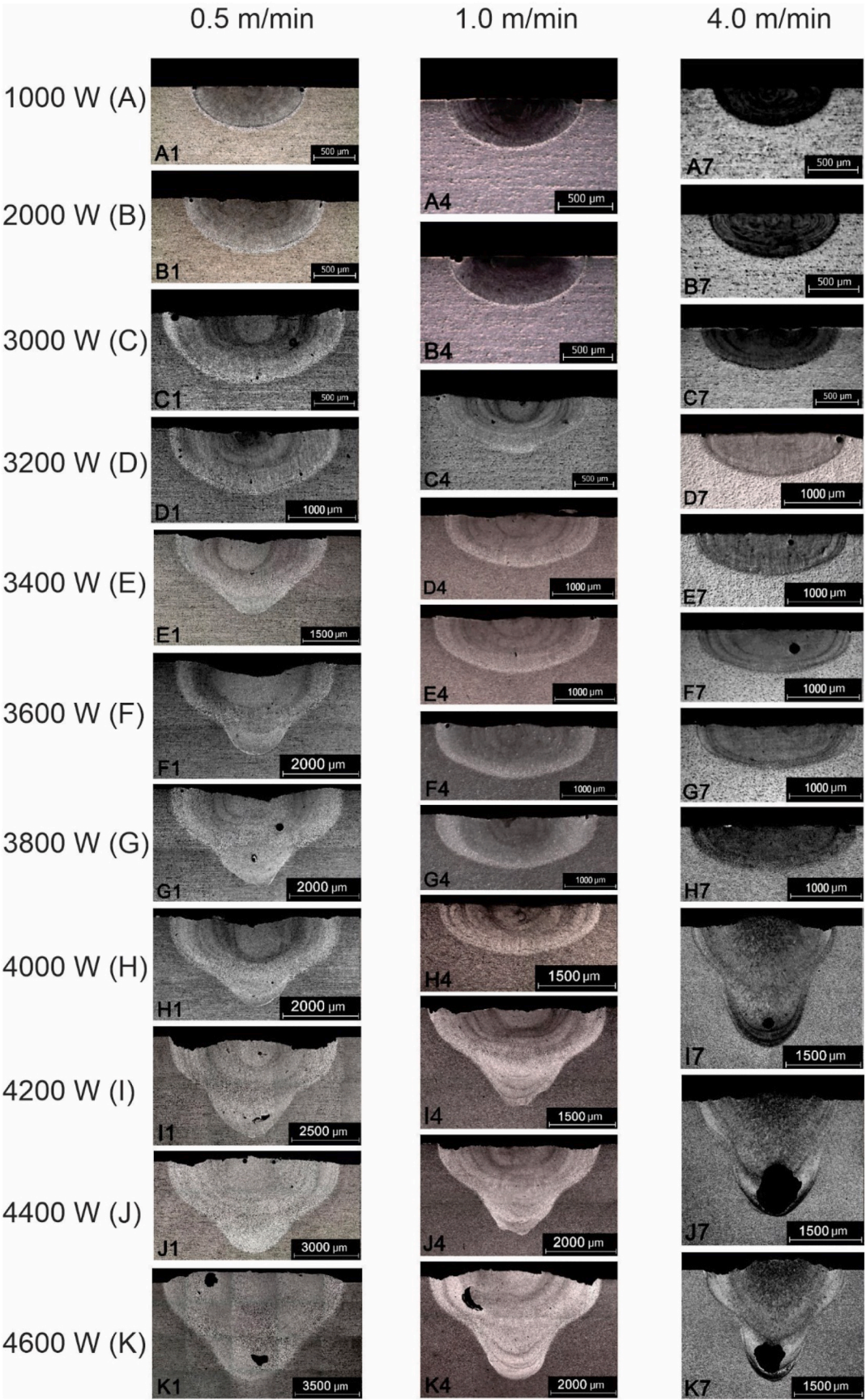


Fig. 3. Macrographs of the weld beads obtained for different scanning speed and power combinations.

**Table 2**  
Best combinations of hyperparameters for each ML technique determined with the GridSearch.

|     | Description                                                  | Parameter                         | Value                                           |
|-----|--------------------------------------------------------------|-----------------------------------|-------------------------------------------------|
| SVR | Tolerance margin                                             | ttr_regressor_estimator_epsilon   | 0.05                                            |
|     | Penalty parameter                                            | ttr_regressor_estimator_C         | 10                                              |
|     | Kernel parameter                                             | ttr_regressor_estimator_gamma     | scale                                           |
| DT  | Maximum depth of the tree                                    | max_depth                         | 8                                               |
|     | Minimum number of samples required to split an internal node | min_sample_split                  | 5                                               |
|     | Minimum number of samples in a leaf                          | min_samples_leaf                  | 1                                               |
|     | Number of features considered at each split                  | max_features                      | None                                            |
|     | Function for evaluating the quality of a split               | criterion                         | squared_error                                   |
|     | Strategy for selecting the split at each node                | splitter                          | random                                          |
|     | Maximum depth of the tree                                    | max_depth                         | 6                                               |
|     | Minimum number of samples required to split an internal node | min_sample_split                  | 2                                               |
| RF  | Minimum number of samples in a leaf                          | min_samples_leaf                  | 1                                               |
|     | Number of features considered at each split                  | max_features                      | sqrt                                            |
|     | Function for evaluating the quality of a split               | criterion                         | squared_error                                   |
|     | Number of trees in the ensemble                              | n_estimators                      | 800                                             |
|     | Bootstrap                                                    | bootstrap                         | True                                            |
|     | Number of neighbors considered                               | knn_n_neighbors                   | 5                                               |
|     | Parameter of the Minkowski distance metric                   | knn_p                             | 1 (Manhattan distance)                          |
|     | Weights (how each neighbor contributes to the prediction)    | knn_weights                       | distance (Closer neighbors have greater weight) |
| ANN | Number of neurons in the first hidden layer                  | nn_model_units1                   | 128                                             |
|     | Number of neurons in the second hidden layer                 | nn_model_units2                   | 32                                              |
|     | Dropout rate applied during training                         | nn_model_dropout                  | 0.2                                             |
|     | L2 regularization factor applied to the weights              | nn_model_l2_reg                   | 0.001                                           |
|     | Optimizer learning rate                                      | nn_model_lr                       | 0.001                                           |
|     | Batch size                                                   | nn_batch_size                     | 32                                              |
|     | Epoch size                                                   | nn_epochs                         | 250                                             |
|     | Clip value                                                   | clipvalue                         | 0.5                                             |
|     | Activation functions                                         | Relu (hidden) and Linear (output) | Relu (hidden) and Linear (output)               |
|     | Optimizer                                                    | Adam                              | Adam                                            |

3.1. Quantitative performance

The performance of the five ML techniques (i.e., SVR, DT, RF, KNN, and ANN) was evaluated on the unseen test set using the coefficient of determination ( $R^2$ ), mean squared error (MSE), and mean absolute percentage error (MAPE) metrics, as detailed in Table 3 and Fig. 4. All techniques demonstrated a strong correlative ability, achieving  $R^2$  values exceeding 0.9 for both bead width and penetration depth. However, the  $R^2$  metric, while indicative of a general trend, is often insufficient for robust selection in complex industrial processes, where the magnitude and practical significance of prediction errors are paramount.

A more discerning evaluation using MAPE reveals a clear performance hierarchy. For bead width prediction, the DT technique achieved the lowest MAPE of 4.49%, closely followed by KNN at 4.68%. For the more challenging task of predicting penetration depth, KNN emerged as the top performer with a MAPE of 8.35%, followed by RF at 8.95%.

The most striking result from this quantitative analysis is the significant underperformance of the ANN, which yielded the highest MAPE values for both outputs: 12.54% for width and 17.88% for penetration depth. This outcome is counterintuitive, as ANNs, with their multi-layered architecture and nonlinear activation functions, are renowned for their capacity as universal function approximators, often excelling in modeling complex, nonlinear physical phenomena where other models falter [41]. This apparent paradox (where a simpler, classical algorithm decisively outperforms a more powerful and complex one) serves as the central question for the subsequent discussion. The explanation lies not in the inherent limitations of ANNs, but rather in the specific correlation between model complexity and the unique characteristics of the dataset collected in this study.

3.2. The impact of the dataset characteristics

The performance disparity between the techniques can be effectively explained in terms of the bias-variance tradeoff, a fundamental concept in supervised learning that describes the relationship between a model's complexity and its ability to generalize to new, unseen data [42]. The dataset used in this study, with only 99 total samples, represents a "small data" or "data-starved" environment, a common challenge in industrial research where experiments are costly and time-consuming. In such a regime, the bias-variance tradeoff becomes the dominant factor in model selection.

ANNs are characteristically low-bias, high-variance models. Their architectural complexity (in this case, featuring hidden layers with 128 and 32 neurons) provides immense flexibility to learn complex relationships within the data. While this is an advantage with large datasets, it becomes a significant liability with limited data. The ANN is susceptible to overfitting; its high variance means it is highly sensitive to small fluctuations and noise in the training set. It learns not only the underlying physical process but also the random experimental scatter, creating a complex function that fits the 80% training data exceptionally well but fails to generalize to the 20% test set, resulting in poor predictive accuracy. That is, deep ANNs are prone to overfit in small datasets.

In contrast, the KNN algorithm is a non-parametric, "lazy learning" method whose complexity is governed by the number of neighbors,  $k$ . With an optimized  $k = 5$ , the KNN technique makes predictions by locally averaging the outputs of the five closest data points in the feature space. This averaging mechanism inherently smooths out predictions and makes the model less sensitive to individual noisy data points, resulting in a model with lower variance. While this simplicity may introduce more bias (i.e., the model cannot capture a highly complex global function), this tradeoff is highly advantageous in a low-data context. The model forgoes capturing every nuance of the training data in favor of a more stable and generalizable function, leading to superior performance on the test set.

**Table 3**  
Performance metrics of bead width and penetration depth on the test set for the five trained ML techniques.

|     | R <sup>2</sup><br>Width | R <sup>2</sup><br>Penetration Depth | MSE<br>Width | MSE Penetration Depth | MAPE Width (%) | MAPE Penetration Depth (%) |
|-----|-------------------------|-------------------------------------|--------------|-----------------------|----------------|----------------------------|
| SVR | 0.9427                  | 0.9473                              | 0.2263       | 0.2056                | 6.05           | 17.26                      |
| RF  | 0.9762                  | 0.9216                              | 0.0939       | 0.1493                | 5.30           | 8.95                       |
| DT  | 0.9832                  | 0.9287                              | 0.0662       | 0.2300                | 4.49           | 10.37                      |
| KNN | 0.9819                  | 0.9296                              | 0.0715       | 0.1341                | 4.68           | 8.35                       |
| ANN | 0.9139                  | 0.9161                              | 0.2776       | 0.1071                | 12.54          | 17.88                      |

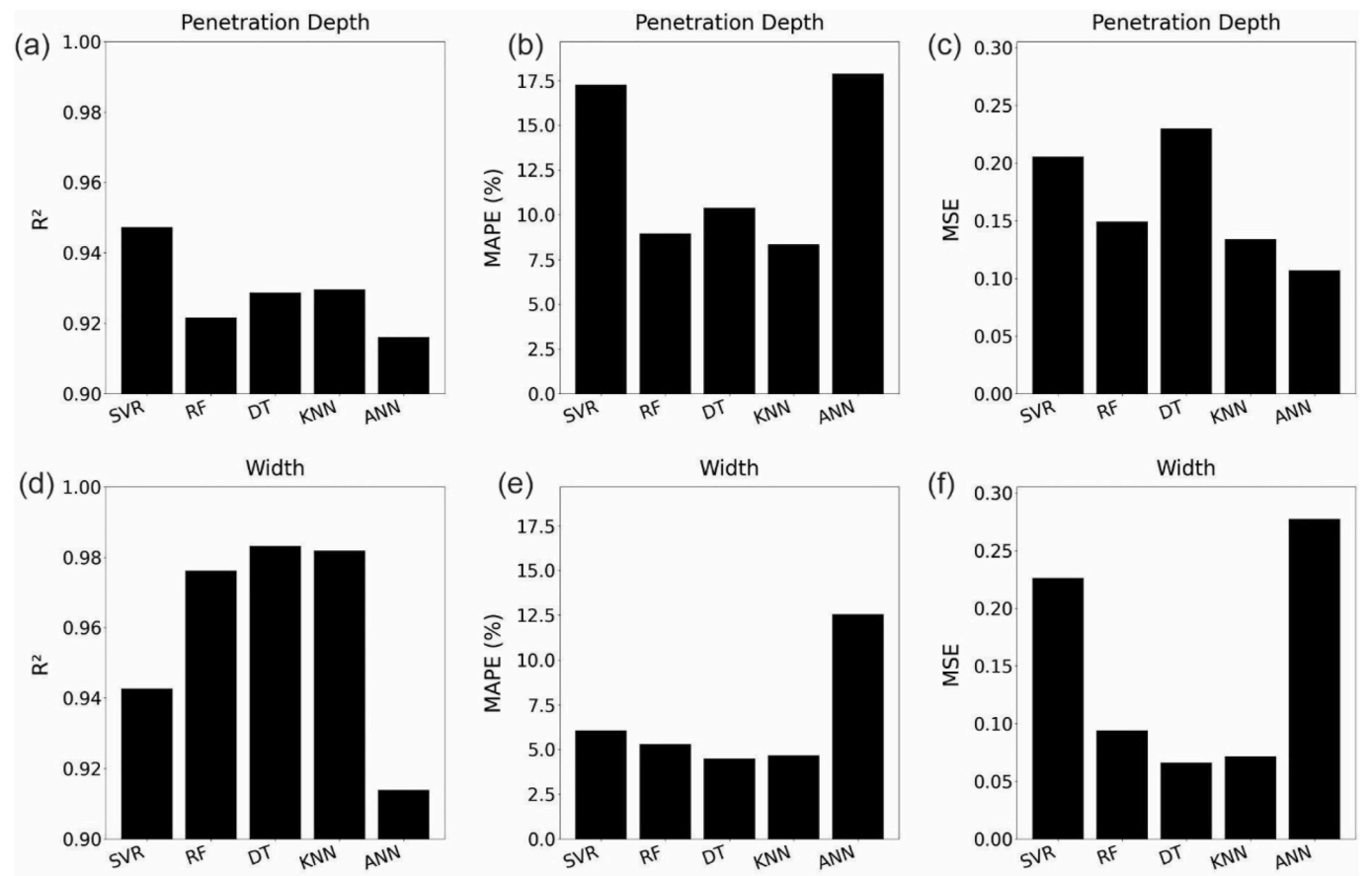


**Fig. 4.** Performance metrics of bead width and penetration depth on the test set for the five trained ML techniques. (a)  $R^2$  penetration depth. (b) MAPE penetration depth. (c) MSE penetration depth. (d)  $R^2$  width. (e) MAPE width. (f) MSE width.

Finally, the tree-based techniques, DT and RF, occupy a middle ground. A single DT is also a high-variance model, prone to overfitting. However, the RF algorithm mitigates this by employing bootstrap aggregating (bagging), an ensemble technique that averages the predictions of many individual trees trained on different subsets of the data. This averaging process is a powerful variance-reduction strategy, which explains why RF consistently ranks as a top-three performer for both outputs in our study. The strong performance of the single DT technique for width prediction suggests that the relationship for this specific output may be well-approximated by its piecewise, axis-aligned partitioning of the feature space.

**3.3. Model selection: predictive accuracy vs. physical plausibility**

While MAPE metrics place DT and KNN as the top candidates, a final selection requires moving beyond numerical scores to evaluate the physical plausibility of the models' predictions. This is crucial for developing a tool that not only predicts accurately but also reflects the continuous nature of the underlying manufacturing process. In this

regard, Fig. 5 directly compares the prediction curves for bead width generated by the DT and KNN techniques across the full range of laser power with the experimental data for the scanning speed of 0.5 m/min. It should be noted that Fig. 5 also compares individual experimental measurements with the corresponding model predictions, rather than averaged values obtained from repeated experiments. Each point in the figure represents a single weld bead measurement, and the experimental variability is therefore inherently reflected by the scatter of the data points themselves.

The DT technique (Fig. 5a), despite achieving the lowest MAPE for width, produces a characteristic step-like output. This behavior is a direct artifact of its algorithmic structure, which recursively partitions the input feature space into a series of discrete, hyper-rectangular regions. Each terminal leaf of the tree corresponds to one such region and assigns a single, constant prediction value to all points that fall within it. While this piecewise-constant approximation can yield high metric scores on a sparse test set, it is fundamentally incongruous with the physics of laser welding. The process is governed by continuous phenomena of heat transfer and fluid dynamics, where a continuous change

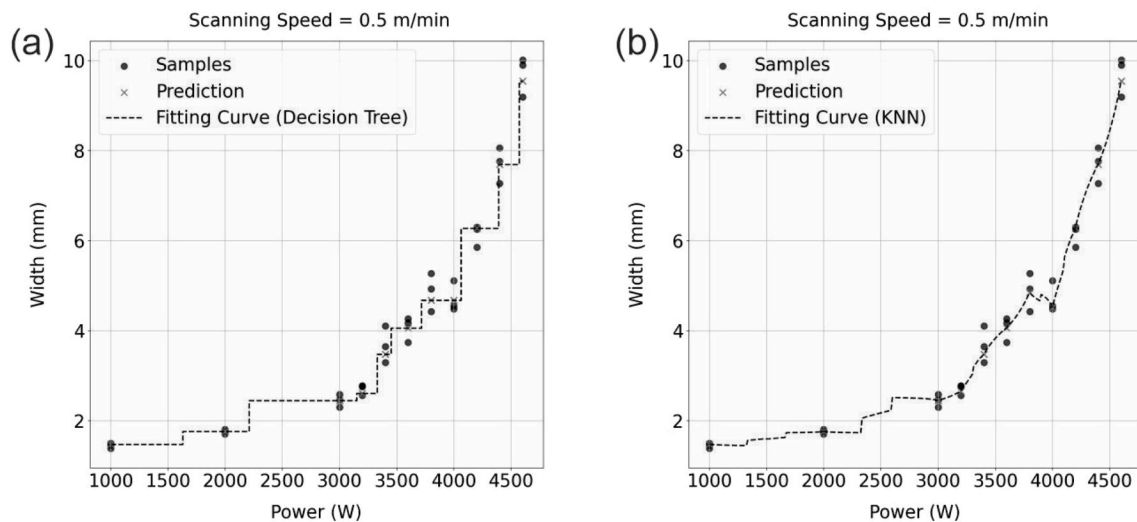


Fig. 5. Comparison between experimental data and predicted results with DT (a) and KNN (b).

in an input parameter like laser power should, in principle, result in a continuous change in the output geometry. The sharp discontinuities generated by the DT technique are not representative of this physical reality and limit its utility for interpolation or for generating a scientifically sound process map.

In contrast, the KNN technique (Fig. 5b) generates smooth, continuous prediction curves that align well with physical intuition. This superior qualitative performance, combined with its excellent MAPE scores, makes it the most recommended technique for the predicted weld bead geometry of 5083-H112 aluminum alloy. The unexpected success of KNN, an algorithm sometimes outperformed in other welding studies [21,25,26], can be attributed to its "lazy learning" approach, which is exceptionally well-suited to the specific challenges of this dataset. KNN does not attempt to learn a single, global function. Instead, for each prediction, it considers only a local neighborhood of the most similar data points (the 'k' nearest neighbors) from the training set. This local approximation strategy provides two key advantages here:

1. **Handling sharp non-linearity:** It effectively captures the abrupt change in process behavior associated with the transition between welding regimes (conduction and keyhole) by drawing upon neighbors from only the relevant local region of the feature space, without being biased by data from the other regime.

2. **Robustness to noise:** The hyperparameters chosen via cross-validation ( $k = 5$  and weights = 'distance') create a robust local averaging mechanism. By considering five neighbors and giving more weight to those that are closer, the model naturally smooths out the impact of random experimental variations or "low repeatability" noted in the dataset, a known strength of KNN when  $k$  is chosen appropriately. This results in the generation of a stable, representative trend that is both metrically accurate and physically plausible.

#### 3.4. Model validation

With the KNN technique selected, its predictions can be further analyzed by using the welding physics to validate its ability to learn meaningful process-property relationships. This analysis connects the model's mathematical outputs to the complex heat transfer and phase change phenomena governing the formation of the weld bead.

Fig. 6 shows the feature's importance for bead width (a) and penetration depth (b), considering power and scanning speed as input parameters and using the KNN algorithm.

The permutation-based feature importance analysis revealed that laser power is the predominant factor in predicting both bead width and penetration depth, showing higher average values compared to scanning speed. For bead width, although both variables contributed, power proved to be more relevant, indicating greater model sensitivity to this

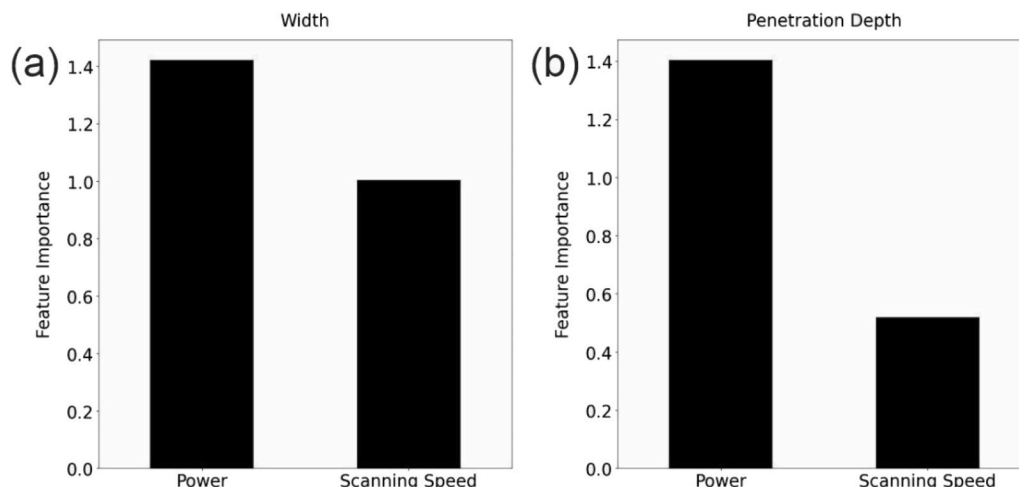


Fig. 6. Feature importance for width (a) and penetration depth (b).

parameter. For penetration depth, the dependence on power was even more pronounced, with scanning speed playing a secondary and less influential role. This result is consistent with the findings of a sensitivity analysis reported in a previous study [4], which, although referring to arc welding, demonstrates a general trend.

The ultimate goal of an ML technique is to generalize its learned knowledge to make accurate predictions on new data. In this sense, Fig. 7 shows a scatter plot for KNN test samples, with actual width (a) and penetration depth (b) values on the y-axis and predicted values on the x-axis. The dashed diagonal line represents the ideal prediction, and the closer the data points lie to this line, the better the model's performance. The  $R^2$  value was 0.982 for width and 0.930 for penetration depth. This quantitatively confirms that the technique has successfully learned the underlying input-output relationships of the process, rather than simply memorizing the training data.

Fig. 8 shows the fitting curves for width and penetration depth obtained with the KNN algorithm, considering all scanning speeds (0.5 m/min, 1.0 m/min, and 4.0 m/min).

In general, both bead width and penetration depth increase with higher laser power, although with a strongly nonlinear behavior. For bead width (Fig. 8(a)–(c), (e)), at low power levels (<2500 W) the values remain close to 2 mm, whereas from ~3000 W onward, a sharp increase is observed. The maximum width (~10 mm) was obtained at the lowest scanning speed (0.5 m/min), while at the highest scanning speed (4.0 m/min), the width was limited to approximately 3 mm. This result confirms the strong influence of scanning speed in reducing the heat input per unit length, thereby restricting bead widening.

A similar trend is observed for penetration depth (Fig. 8(b)–(d), (f)). At low power conditions, penetration is minimal (<1 mm), but from 3500 W onward a rapid increase is observed, reaching values above 5 mm at 0.5 m/min. At 4.0 m/min, however, even under high power levels, penetration did not exceed ~2.5 mm.

The practical output of this validated model is presented in the form of prediction maps (Fig. 9), which visualize the predicted bead width and penetration depth across the entire investigated parameter space. The prediction maps are intentionally presented in order to provide a global and unbiased view of the process behavior, rather than restricting the analysis to a predefined geometry window. This choice allows the identification of multiple potentially suitable operating regions depending on the application requirements, and avoids embedding application-specific constraints into the model visualization.

Regions of the same color indicate similar values. For bead width, within the range of 1.0–2.5 m/min at 4500 W, the predicted values are very close, suggesting low sensitivity to scanning speed at this power level. Similarly, for penetration depth, between 1.0 and 4.0 m/min at

4500 W, the variations with scanning speed are minimal. This behavior is consistent with the feature importance analysis, which indicated a stronger influence of laser power than scanning speed on both responses.

These maps serve as a powerful data-driven predictive model of the welding process, enabling engineers to move beyond time-consuming and resource-intensive trial-and-error experimentation. For instance, an engineer can use these maps to perform multi-objective optimization: identifying a process window that achieves a required penetration depth (e.g., for structural integrity) while simultaneously maximizing welding speed (to increase productivity) and minimizing laser power (to reduce energy consumption and operational costs). The maps also reveal regions of process stability; the observation that penetration depth becomes less sensitive to scanning speed at high power levels (Fig. 9b) identifies a robust operating regime where minor fluctuations in speed will not significantly compromise weld quality. Naturally, with these maps, it is possible to select the most suitable parameters for a given application, whether as a basic requirement in welded structures [13] or for optimization and correlation with ductility [14].

Further work will extend the present approach to include a detailed microstructural characterization of the welds, aiming to correlate the predicted processing windows with microstructural features such as porosity and grain size.

#### 4. Conclusions

The present study aims to analyze and compare the predictive performance of five widely used machine learning regression techniques, i. e., SVR, DT, RF, KNN, and ANN, for estimating weld bead width and penetration depth from scanning speed and welding power in laser welding of AA5083-H112 aluminum alloy. A challenging experimental dataset was employed, characterized by limited size, low repeatability at certain points, and the presence of discontinuities associated with the transition from conduction to keyhole mode. Based on the obtained results, the following conclusions can be drawn:

- The KNN algorithm was the most recommended for predicting bead width and penetration depth. This was due to its low MAPE (4.68% for width and 8.35% for penetration depth), combined with the generation of smoother curves that consistently followed the increasing trend with power, resulting in more realistic representations of the phenomenon.
- For bead width, the ranking of algorithms based on MAPE, in decreasing order, was DT (4.49%), KNN (4.68%), RF (5.30%), SVR (6.05%), and ANN (12.54%). For penetration depth, the ranking was

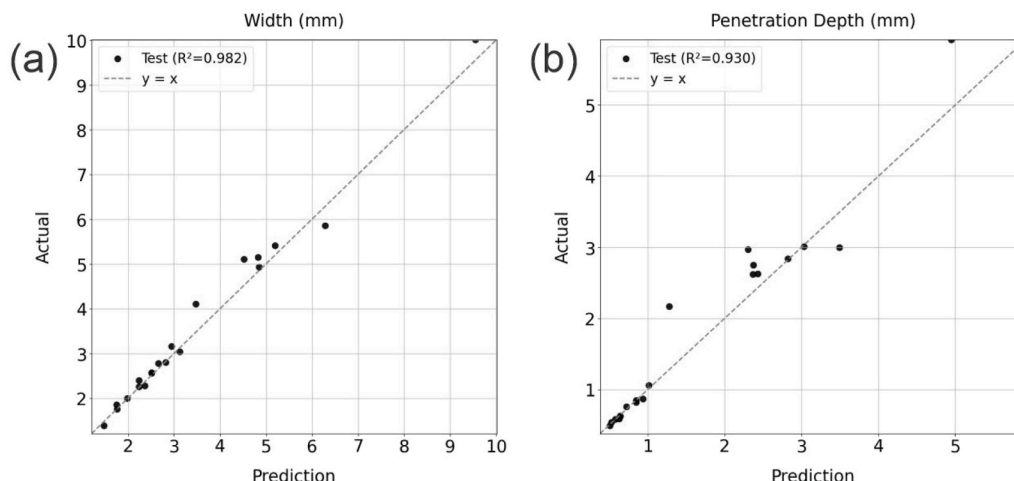


Fig. 7. Scatter plot for KNN test samples showing prediction versus actual values. (a) Width. (b) Penetration depth.

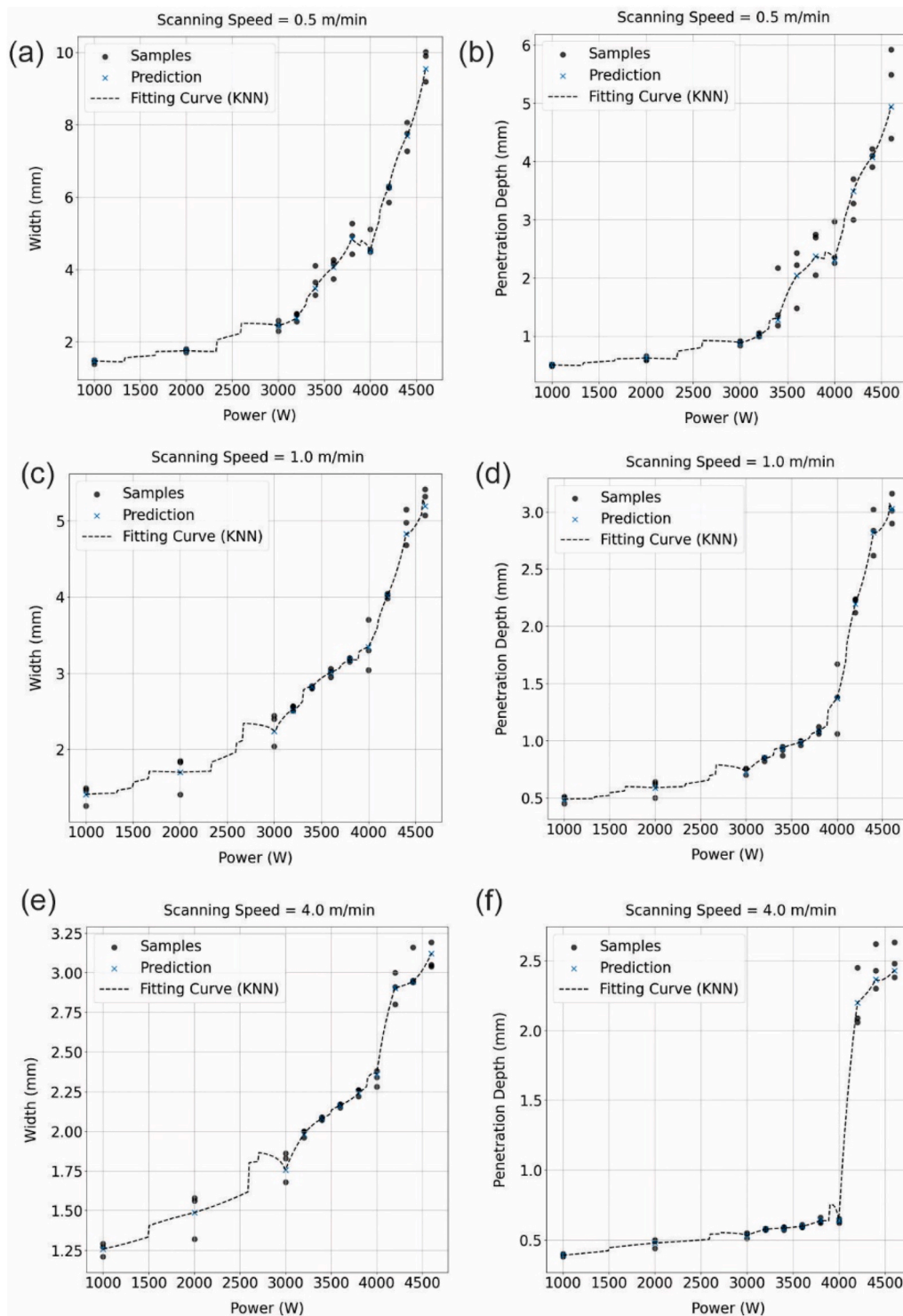


**Fig. 8.** Fitting curves considering the KNN algorithm. (a) Width and 0.5 m/min. (b) Penetration depth and 0.5 m/min. (c) Width and 1.0 m/min. (d) Penetration depth and 1.0 m/min. (e) Width and 4.0 m/min. (f) Penetration depth and 4.0 m/min.

KNN (8.35%), RF (8.95%), DT (10.37%), SVR (17.26%), and ANN (17.88%).

- All techniques achieved  $R^2$  values above 0.9, indicating strong predictive performance even with a limited dataset. The low errors obtained for both width and penetration confirm that the models were able to capture the main physical relationships of the process. Although this is a positive outcome, it indicates that this metric alone is not decisive for performance evaluation.

- The feature importance analysis revealed that laser power is the predominant factor in predicting both bead width and penetration depth, showing higher average values compared to scanning speed.
- The prediction maps generated in this study provide a means to select the most suitable parameters for a given application, with respect to bead geometry, within the domain of 1000–4600 W and 0.5–4.0 m/min.

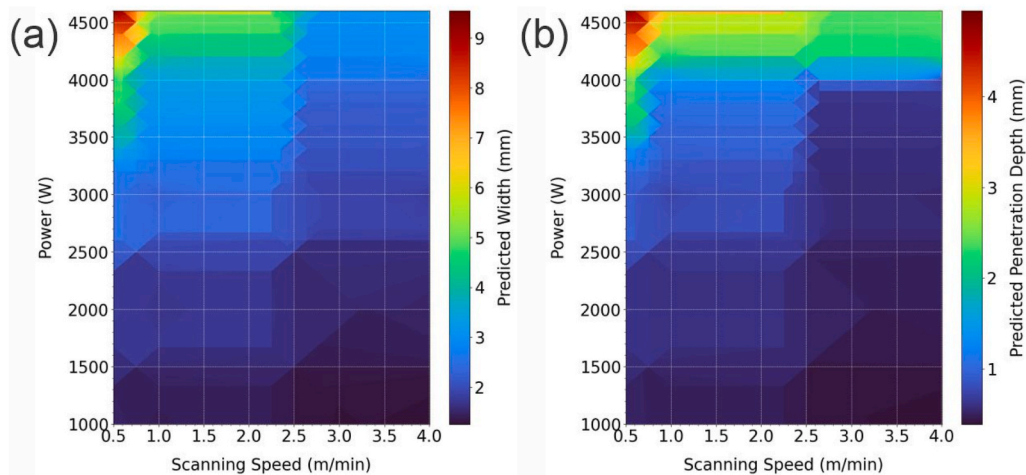


Fig. 9. Prediction maps of the KNN technique for width (a) and penetration depth (b) as a function of power and scanning speed.

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## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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