Materials Research Proceedings 41 (2024) 300-307 https://doi.org/10.21741/9781644903131-34

Artificial intelligence approaches for enhanced coating performance

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Keywords: Cold Spray, Deep Learning, Genetic Algorithms

Abstract. Cold spray (CS) is an innovative manufacturing technology designed to produce metallic layers on diverse materials. This process involves propelling metallic particles at supersonic speeds using pressurized gas, causing them to impact the target surface and achieve adhesion through mechanical interlocking between the powders and the substrate. Integrating Artificial Intelligence (AI) techniques can enhance the understanding and quality of this additive manufacturing process. This work focuses on predicting the characteristics of particle deformation upon collision by exploring multiple Machine Learning (ML) and Deep Learning (DL) techniques with the aim of identifying the most suitable approach. The used dataset is mixed data, composed of experimental data and FEM data, generated by Finite Element models (FEM). The input parameters for the model are categorized into three macro-categories: process, powder, and substrate. The research aims to forecast particle behavior through this multidimensional approach and contribute valuable insights for optimizing the cold spray manufacturing process by applying DL methodologies.

Introduction

As an innovative production technique, cold spray stands out for its capability to deposit metallic layers onto diverse materials, unlocking possibilities for creating robust and firmly adherent metal coatings. The broad applications span various industries, from aerospace to manufacturing and beyond [1]. A crucial aspect of exploring the potential of cold spray lies in conducting comprehensive coating studies to understand the behavior and performance of these coatings on different surfaces or objects. The intricate mechanisms of bonding formation and deposit strength are influenced by numerous factors [2]. Traditionally, material characterization has relied on manual efforts, often hindered by the need for a centralized database containing information on material properties. This bottleneck can pose challenges, mainly when performing FEM analyses [3] on newly introduced materials and substrates. Predicting the ultimate characteristics of a coating is a complex task. This complexity arises from the intricate interplay of numerous factors. These factors encompass the metallic powder's inherent properties, the polymeric substrates' characteristics, and the specific spraying parameters selected for the process. The challenge lies in the intricate synergy of these elements, making it presently tricky to forecast the behavior of metallic particles upon impact with diverse substrates precisely. The intricate nature of these interactions necessitates a comprehensive understanding of material properties, substrate dynamics, and process conditions, highlighting the current limitations in accurately predicting the outcomes of such interactions. Addressing these challenges requires innovative approaches and

advanced modeling techniques to enhance our ability to anticipate and control the behavior of metallic particles during the coating process.

Recognizing this limitation, the current study focuses on leveraging deep learning and broader artificial intelligence techniques. This study uses DL models to analyze a comprehensive material dataset comprising experimentally validated results, and genetic algorithms are employed to design the network architecture. The objective is to enable accurate predictions of FEM results across multiple materials, even those not initially included in the original dataset. The input parameters incorporated into the model are systematically grouped into three categories: process parameters, powder parameters, and substrate parameters. The selected output parameters, chosen with precision to capture the fundamental traits of the coating, are flattening and penetration. These parameters are significant as they directly influence the coating's uniformity and adhesion characteristics. This research aims to pioneer the integration of DL models with GAs to achieve two main objectives:

- Firstly, the focus is on developing a sophisticated tool that predicts and enhances the characteristics of coatings. Through the iterative optimization facilitated by GAs, the DL models can refine their predictions and guide the enhancement of coating properties, thus advancing the capabilities of coating technologies;
- Secondly, the research endeavors to expand the scope of automation in the coating process by training additional DL models. The goal is to support the capacity for complete automation in coating applications.

Materials and methodologies

Input and output parameters. The input parameters for the implemented strategies can be categorized into three main groups: impact velocity, encompassing various process parameters such as temperature, pressure, and stand-off distance; *powder parameters* (Yp), which, for metallic coatings on polymeric substrates, can be summarized by the yield strength of the powder material; and *substrate parameters* (Ys), that for polymeric substrates which are only deformed by the impact of the particles at low temperatures, can be characterized by the yield strength of the substrate material. The latter also considers the presence of fibers, which, when appropriately positioned beneath a matrix layer at least comparable in size to the powders, solely enhance the substrate stiffness, leading to a variation in yield strength. The output parameters under consideration include the particle *penetration depth* and *flattening*, measured by analyzing SEM micrographs of the coatings. Penetration depth refers to the extent to which a particle can traverse or penetrate a material or surface and evaluates the height of the particle upon the impact [Hs0]. The penetration depth was defined as $Hs\ [\%] = \frac{(Hs_0 - Hs)}{Hs}\ 100$. To assess the degree of powder flattening, the examination focused on the top surface of the coating. Using Image J software, the mean radius of the particles following a collision with the substrate (r) was measured. The percentage of particle flattening was calculated $r/r_0\ [\%] = \frac{(r-r0)}{r0} 100$, where r_0 represents the mean radius of the particle before the impact. As regards the formation of the dataset, the ones used in this study were created using both finite element method (FEM) simulations and experimental data. The first training dataset consisted of 30% experimental data and 70% FEM data, which were combined. Further information on the FEM analysis performed is presented in previous works of the authors [9]. The second dataset only included FEM data. The test dataset for both models only consisted of experimental data, for both FEM and experimental dataset, ABS, PEEK, and PA66 were considered as substrate materials, while copper, aluminum, steel, and titanium were the powders employed. LPW South Europe provided all the spherical powders used in the deposition process. A low-pressure cold spray equipment called DYCOMET was used for the depositions. Air was used as the carrier gas based on previous research indicating no significant

differences when using other carrier gases. The samples were positioned on a platform, and a spraying gun attached to a robot (HIGH-Z S-400/T-CNC-Technik) was used remotely to spray the substrates perpendicularly. Table 1 highlights the process parameters and characteristics of the powders used in the experiments.

Table 1. CS parameters employed for the experiments

Inlet Gas temperature [°C]	100 - 400	100 - 400	100 - 400
Standoff distance [mm]	10 - 4	10 - 4	10 - 4
Inlet gas pressure [MPa]	0.5 - 0.6	0.5 - 0.6	0.5 - 0.6
Gun traverse speed [mm s^{-1}]	7.5	7.5	7.5

DL models and Genetic algorithm approach

GAs are optimization techniques inspired by the principles of evolutionary theory in biology. These algorithms mimic the process of natural selection, evolution, and genetic recombination observed in living organisms. By emulating the mechanisms of genetic variation, reproduction, and survival of the fittest, genetic algorithms strive to find optimal solutions to complex problems. This computational approach involves the generation of diverse solutions, their evaluation based on a defined fitness criterion, and the evolution of increasingly refined solutions over successive generations. Genetic algorithms have proven effective in solving various optimization challenges across various fields, leveraging the inherent adaptability and efficiency inspired by the biological processes that govern evolution [4]. GAs aim to construct a population of potential solutions for a given problem, employing a fitness function to evaluate the merit of each candidate solution. The algorithm then identifies the best solutions to form a new population, perpetuating this iterative process and refining the solutions. Essential operations characterize each GA iteration:

- *initialization:* the algorithm initiates by randomly populating the pool of potential solutions;
- *selection*: optimal parents are chosen from the existing population based on their fitness.
- *crossover*: genetic material from the current population is recombined to generate novel solutions;
- *mutation*: random changes to the genetic material are introduced to prevent the algorithm from getting trapped in local optima, fostering new genetic variations;
- *evaluation*: the fitness of each solution is compared to the target, which could be based on factors such as the number of generations or the fitness of the best solution;
- *replacement*: the current population is replaced with a new generation of solutions, and this process is repeated until a satisfactory solution is found or after several generations.

In this scenario, we used the GAs and their related terminology and operations to design the architecture of the network, rather than optimizing the network's hyperparameters. A neural network is a computational model inspired by the structure and functioning of the human brain. It consists of interconnected nodes, often called neurons or artificial neurons, organized into layers.

The fundamental building blocks are the input layer, hidden layers (if any), and the output layer. In a neural network, information flows through the network feedforward, with each node connection having an associated weight. The network processes input data through these weighted connections, applying activation functions at each node to introduce non-linearity and complexity. Neural networks can learn from data through training, where the weights are adjusted based on the error between predicted and actual outputs. This learning ability allows neural networks to generalize patterns and predict or classify new, unseen data. The entity E_i is represented as a vector $E_i = \{F_1, \ldots, F_m\}$ comprising *m* features. Each feature F_j of E_i indicates a gene. The Genome of E_i encompasses the complete set of genes. The Population at time t, denoted as $P(t) = \{E_1, \ldots, E_n\}$, is the collection of entities. To achieve an adequately expanded network architecture in the experiment, the initial genome size was set to ten, ensuring the presence of the minimum layers needed for executing a CNN. Each gene corresponds to a specific Matlab CNN network layer: input, dropout, batch norm, cross-chan norm, 2D-convolution, RELU, softmax, and Fully Connected. Chromosomes are represented by arrays, with each cell indicating the presence or absence of a characteristic (feature) within the entity. A feature represents one of the CNN layers. Activation of a feature (array cell) incorporates the associated layer into the network, while inactivity excludes the layer when the feature is not expressed. Due to the operation mutation, each feature F_j may or may not be expressed by E_i, resulting in the presence of both silent and expressed genes. In this context, the training was conducted using a 5% validation and 10% test cross-validation approach to assess the performance of the models and ensure robustness and generalization. This involved the division of the dataset into multiple subsets, with 5% of the data reserved for validation and 10% for testing.

To assess the effectiveness of the DL approaches, we computed several performance metrics, including the Root-mean-square error (RMSE) [5], R-squared [6], Mean Squared Error (MSE) [7], and Mean Absolute Error (MAE) [8]. RMSE is derived from the squared mean error and is a metric sensitive to outliers. R-squared serves as a goodness-of-fit metric for linear regression models, indicating the proportion of variance in the dependent variable explained by the independent variables. It quantifies the strength of the association between the model and the dependent variable. MSE reflects the mean squared difference between observed and estimated data values. On the other hand, MAE signifies the distance between predicted and measured values. Lower values for these metrics indicate higher model accuracy.

Results and Discussion

In this section, we reported the results of the mixed data (FEM and experimental data). The execution of GAs disclosed the existence of two straightforward NN architectures. Specifically, for the flattening, the best network was a Wide Neural Network (WNN). In contrast, for the penetration, the best results were achieved by a Trilayered Neural Network (TNN), as reported in Table 2 and 3. In Fig. 1 and Fig. 2, we depicted the plot of the results.

The WNN refers to an artificial neural network architecture that typically has fewer hidden layers but a substantial number of nodes in each layer, providing it with the capacity to capture a wide range of features and relationships within the data. In this context, the TNN is formed by one fully connected layer and a ReLU activation function. The TNN is a form of artificial neural network, also known as a single-layer perceptron. It consists of three layers: an input layer, which receives the initial data; a hidden layer, which processes the input data using weighted connections and activation functions; and an output layer, which produces the final results. The obtained TNN comprises three fully connected layers and a ReLU activation function. The selected NN models demonstrate enhanced penetration values on the validation set but decreased penetration performance on the test set. On the other hand, on the test set, WNN reached the best performance. Additional studies and model evaluation metrics are required to understand this behavior.

Table 2. Results for flattening on validation and test sets

Model: WNN	**RMSE**	**R-Squared**	**MSE**	**MAE**
Validation set	2.48	0.75	6.16	1.67
Test set	0.73	0.92	0.54	0.51

Table 3. Results for penetration depth on validation and test sets

Model: TNN	**RMSE**	**R-Squared**	**MSE**	**MAE**
Validation set	0.80	0.96	0.64	0.49
Test set	2.57	0.60	6.64	1.46

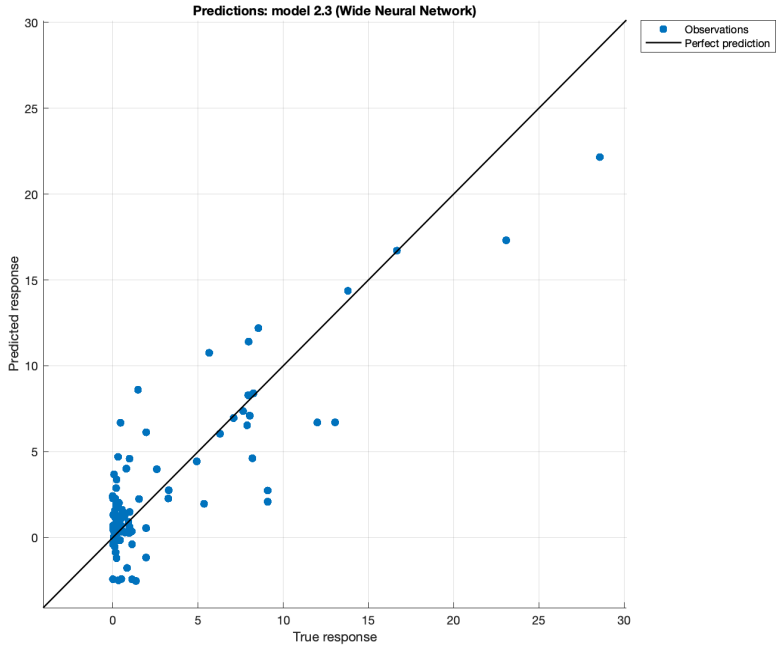

Fig. 1. Performance for the flattening prediction for mixed data

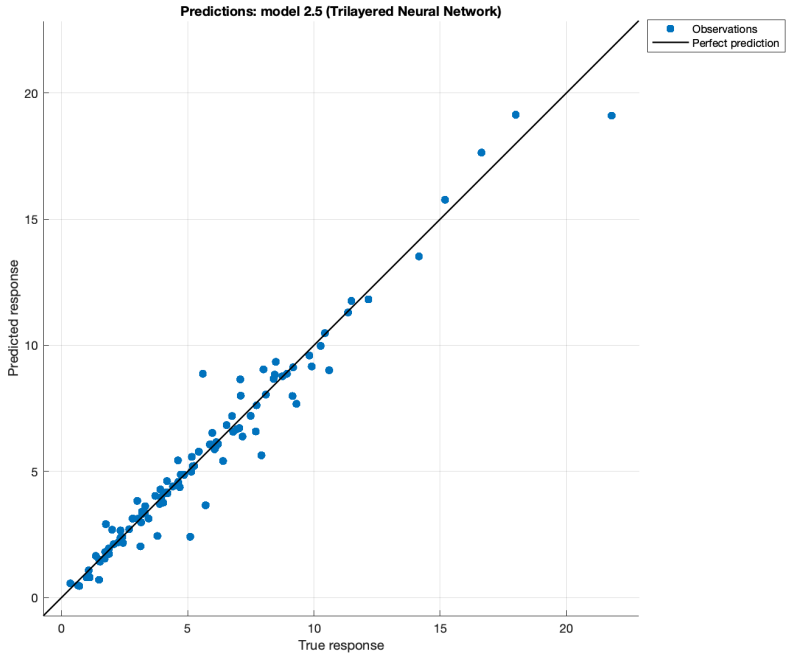

Fig. 2. Performance for the penetration prediction for mixed data

In this scenario, DL can contribute to expediting finite element analyses, a process known for its resource-intensive computing requirements. Additionally, DL enables predictions for novel combinations of materials, eliminating the necessity for running extra simulations. This not only enhances computational efficiency but also broadens the scope of material analysis by providing insights into unexplored configurations, thus showcasing the versatility and potential of machine learning in the domain of FEM analyses.

Comparison with our previous work

Our previous work tested machine learning (ML) techniques on mixed data. The best models were NN for the penetration on the test set and LR for the flattening prediction, as reported in Table 4 [9]. In this previous work, our results showed high performance for the penetration value and their decrease for flattening prediction, as confirmed in this research.

Table 4. Results for flattening and penetration on test set with ML techniques

Models	**RMSE**	**R-Squared**	**MSE**	**MAE**
LR	1.83	0.90	3.36	1.45
NN	0.58	0.96	0.34	0.41

Table 5. Comparison of the models

Output	*Models*	RMSE	R-Squared	MSE	MAE
Flattening	***LR***	1.83	0.90	3.36	1.45
	WNN	0.73	0.92	0.54	0.51
Penetration	***NN***	0.58	0.96	0.34	0.41
	TNN	2.57	0.60	6.64	1.46

In Table 5, we compared the results of the previous work and the approach presented in this study. WNN achieved a high performance for the flattening of the evaluation metrics. For the penetration, the TNN designed using GA shows worse performance. We graphically represented this comparison in Fig. 3. The best model for penetration prediction is NN. We highlighted the best results for flattening and penetration with the color view in Table 4.

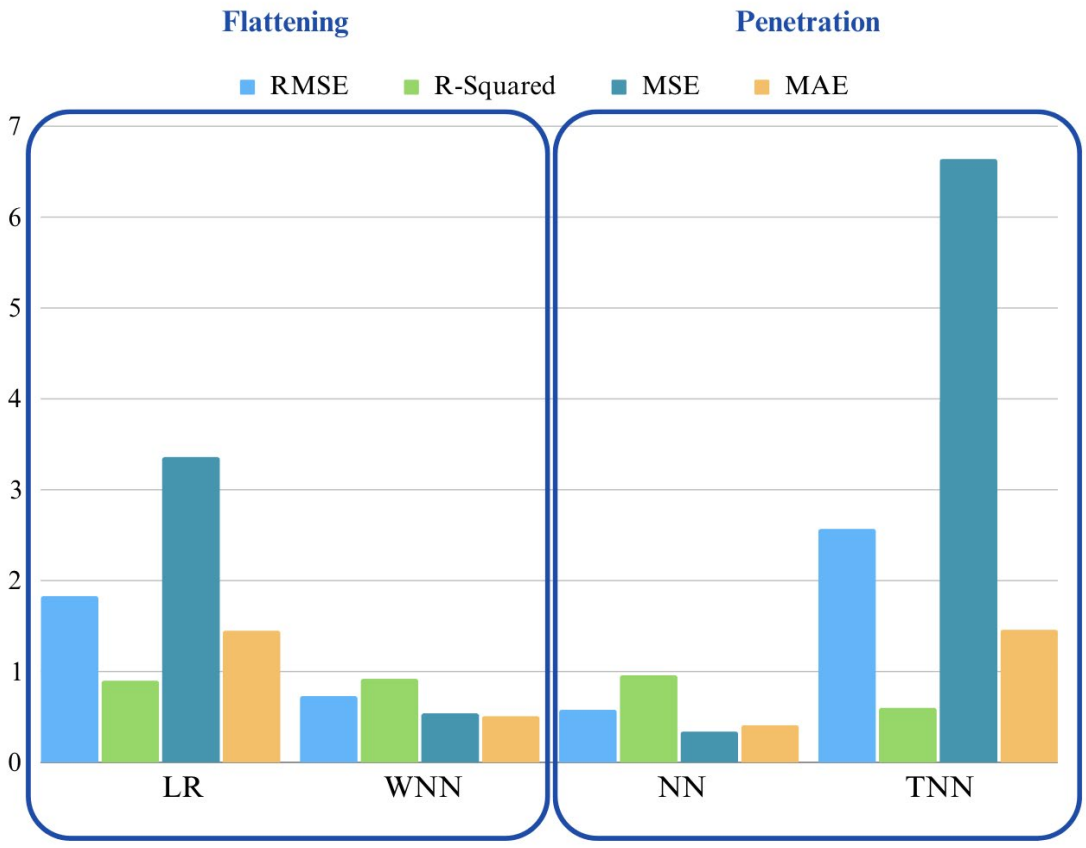

Fig. 3. Comparison of performance

Conclusions

This study applied DL techniques on a mixed dataset for CS to enhance the precision of predicting coating features, such as penetration and flattening, to optimize process efficiency. To design the

architecture of the models, GA is applied to construct the network. The best models are WNN for the prediction of the flattening and TNN for the prediction of the penetration depth. Specifically, WNN can outperform our previous AI models. The conducted experiments demonstrate that DL techniques have the potential to predict optimal parameter combinations, consequently amplifying the efficiency and effectiveness of the coating process. GA can help optimize the design model architectures to minimize the need for manual hyperparameter tuning. This process can be time-consuming and less than optimal. Exploring multi-output regression networks can be considered a potential approach in future works. By employing multi-output regression networks, the model can directly predict multiple outputs simultaneously, potentially enhancing the overall performance and applicability of the system.

Acknowledgments
This study was carried out within the "OPTIMA: depOsition of cold sPray in the realm of green addiTIve manufacturing through construction of MAchine learning models" and received funding from the Research Projects of Significant National Interest (PRIN) 2022 PNRR, project n. D53D23017410001.

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