

Cold Sprayed Metallic Coatings on Fibre-Reinforced Composites: A Machine Learning Approach for the Optimization of the Process

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Abstract. Cold spray additive manufacturing (CSAM) is a promising process for producing metallic layers on different substrates, using powders as a feedstock material. The metallic powders are deposited through pressured gas that reaches supersonic velocities. Due to the low heat input required, as the powders remain in solid-state, this technology is particularly suitable to coat thermo-sensitive materials such as composites. In this scenario, machine learning techniques can be crucial to improve the quality and understanding of this manufacturing process. The aim of this work is to predict the deformation and penetration of a particle upon impact using machine learning techniques in order to assess the properties of the coating. A univariate linear regression method was chosen to verify the feasibility of Theory Guided Machine Learning (TGML) techniques to predict the characteristics of the coating. The training dataset was obtained from both experimental data and computational data. It was confirmed that TGML could be a good route to pursue in order to optimize this process.

Introduction

Due to the necessity of reducing weights and production costs, interest in polymeric materials has grown drastically in recent years [1,2]. In particular, thermosetting polymers became largely employed in many sectors, including aerospace, as they can be used as matrices for fibre-reinforced composite materials [3,4]. However, as environmental issues are gaining growing awareness, the use of thermosets is strongly limited due to the impossibility of reusing and recycling them after the curing process is concluded. For this reason, increasing attention has been directed toward high-performance thermoplastic materials, such as PEEK or PEI, as they are characterized by high resilience, high melting temperature and are completely recyclable [5,6].

Although, many applications are still precluded due to their poor surface characteristics such as low electrical conductivity and poor wear and scratch behaviour. For this reason, surface metallization could be the best path to follow in order to combine the advantages of metals and thermoplastic polymers. Nonetheless, the most commonly used metallization techniques (such as plasma spray or vapour phase deposition), require the melting of the metallic material that loses its initial properties and may damage or cause thermal distortions of the substrate.

In this scenario, Cold Gas Dynamic Spray technique, which exploits kinetic energy and requires temperatures well below the melting point of the metallic particles, could be a suitable alternative for improving the surface properties of polymers [7–9]. This technique is based on the high-speed impact of solid-state metallic particles; the deposition is made possible mainly due to mechanical interlocking between the particles and substrate and no chemical reactions are required.

While this technology has been long studied and applied for applications on metal substrates, the driving mechanisms are still unclear when the substrate is a polymer. In particular, to date, it is not possible to accurately predict the behaviour of the metallic particles upon impact on different substrates: the final characteristics of the coating (such as the powder deformation or penetration depth, which are deeply related to the adhesion of the coating), depend, in fact, on multiple factors such as the characteristics of the metallic powder and the polymeric substrates and the spraying parameters set for the process.

Thus, in the last few years, several computational models have been developed in order to predict the behaviour of a particle impacting a substrate, simulating the operating conditions of Cold Spray process [10–12]. However, as concerns the coating process applied to polymers and composites, to date the very few works have been published [13–15]. Nevertheless, it was not possible to develop a validated physical model to describe the phenomena occurring during the deposition of metallic particles on non-metallic substrates.

In fact, in order to validate those models, it would be necessary to use sophisticated equipment (eg. sensors, high frame-rate cameras) to acquire hundreds of experimental conditions and results. Despite Finite Elements models (FEM) could provide accurate evaluations of the particle conditions upon impact, they require high computation time and effort. A promising solution to reduce the number of required experimental tests could be machine learning. Machine learning solutions are often seen as a black box, where input and outputs are correlated without any information about the process, for this reason, it is necessary to provide accurate data to the learning algorithm [16]. However experimental data are often scarce and fragmented, while computational data (obtained through FE models), despite not having those problems, are often results of a high degree of approximations. Using data obtained from simulations, Machine learning approaches would only be useful to reduce the processing times of pre-existing FE models.

To overcome those issues, a Theory-guided machine learning approach is proposed: not only a combination of virtual and physical data is employed to train the model, but also the physical laws that rule the process are exploited [17]. The theory could be useful to determine the physical features (namely the inputs) to be supplied to the model and to identify the best loss function. This approach would require a lowered number of inputs data to train the model.

In this work, cold spray deposition of copper particles on PEEK substrate is considered, as the deposition of soft copper particles on thermoplastic polymers is well established [18,19]. A univariate linear regression machine learning algorithm is exploited to predict the deformation and the flattening of a copper particle after the deposition is occurred, knowing the impact velocity.

Experimental tests have been carried out with low-pressure equipment to obtain half of the training set and the test set data, and SEM analyses were performed to evaluate the flattening and the penetration depth. An easy analytical model has been developed in order to estimate the impact velocity in the true test conditions, knowing the characteristics of the material and the deformation of substrate and particle after the impact.

A FE simulation of the impact of a copper particle was performed in order to obtain the remaining portion of the test dataset. An analysis of the behaviour of the cost function in both the cases where the penetration depth and the flattening are evaluated.

Materials and Methods

Cold Spray Depositions. Cold spray depositions were carried out in order to build part of the training dataset and the test dataset. Copper spherical powders supplied by LPW South Europe were chosen for the deposition while Polyether-ether-ketone (PEEK) was chosen as a substrate.

The abovementioned depositions were carried out using low-pressure cold spray equipment (DYCOMET). The carrier gas chosen was air, as previous experiments evidenced no significant differences portrayed using different carrier gasses [20].

The specimens were mounted on a platform while the spraying gun (working perpendicularly to the substrates) was mounted on a robot (HIGH-Z S-400/T-CNC-Technik) and remotely controlled. The process parameters were chosen accordingly to previous experiments and literature results and varied accordingly to Table 1.

Table 1 – Process parameters chosen for the deposition

Parameters	Values
Inlet Gas temperature	100 to 400 °C
Standoff distance	10 to 40 mm
Inlet gas pressure	0.5-06 MPa
Gun traverse speed	7.5 mm s ⁻¹

Sixteen different couplings of temperature and standoff values were employed to obtain different values of penetration and deformation of the powders.

After the deposition, the specimen were analysed through SEM microscopy. The top surface of the coating was inspected in order to measure the flattening of the powders, defined as the ratio between the diameter of the particle before the deposition and the diameter of the particle after the deposition measured in the horizontal direction. Image J software was employed to measure the particle diameters after the impact. The flattening values considered is the mean value of the flattening calculated on 3 different 500x500 micron surfaces analysed, as shown in Fig.1.

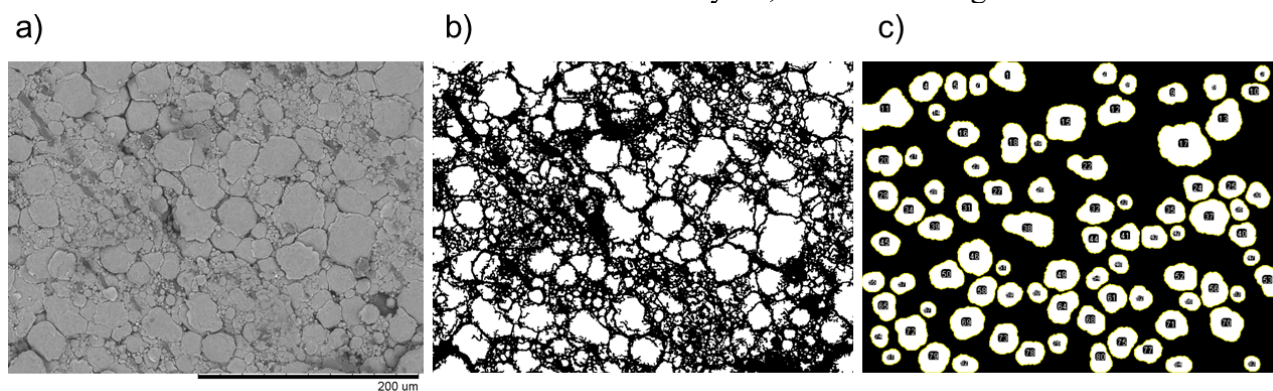


Fig. 1- Estimation of the mean particle deformation. a) SEM micrography of the surface b) Image J manipulation of the micrography c) measure of the particle characteristics through Image J

The specimens were then cut perpendicularly to the top surface to evaluate the penetration depth. This value was measured according to Fig.2.

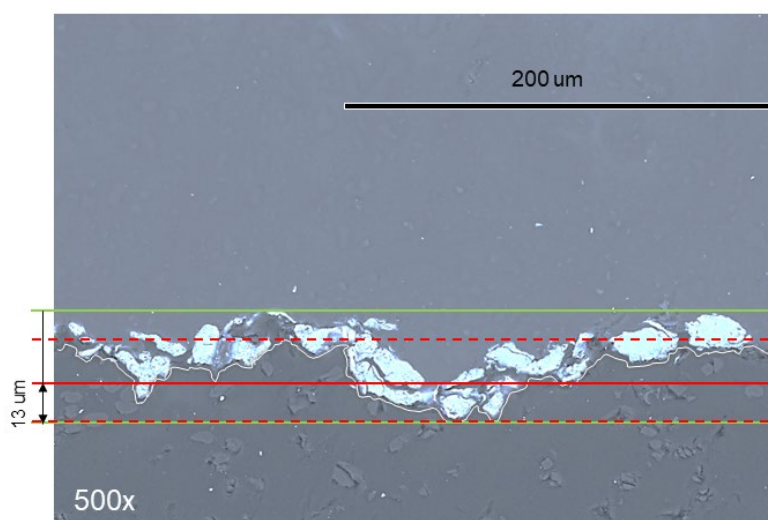


Fig. 2 – Estimation of mean particle penetration depth on SEM micrography of the coating

Theoretical Estimation of the impact velocity. The evaluation of the impact velocity of a single particle in Cold Spray is still one of the main issues with this technology. Some authors in the literature manage to measure it with expensive systems [21] or by using complex and time-consuming fluid dynamic models [22,23].

In order to estimate the impact velocity of the particle without relying on those methods and reducing the calculation times, an analytical energetic-based model to evaluate the single-particle impact behaviour have been developed.

To a material particle, several physical or chemical properties such as volume, density or mass can be ascribed. Due to those properties, the particle owns a certain amount of energy that can be summarized as the sum of kinetic energy, internal energy, thermal energy and potential energy.

Neglecting the potential energy and the internal energy, as those terms are considerably lower in our case study, it is possible to write the particle energy as:

$$Ep = \frac{1}{2}mv^2 + N\frac{f}{2}k_bT$$

Where :

- $\frac{1}{2}mv^2$ is the kinetic energy of the particle in the instant of the impact, with v , impact velocity, m particle mass,
- $N\frac{f}{2}K_B T_p$ is the thermal energy of the particle, with N number of molecules of the particle, f number of degrees of freedom of the system, K_B Boltzmann constant, T_p particle temperature before impact.

After the impact with the substrate, this energy is converted to other forms to obtain adhesion. It is possible to hypothesize that, in the case of a metallic particle impacting on a thermoplastic substrate are heat transfer contribution, plastic deformation of the substrate and plastic deformation of the particle.

As for the first contribution its calculation is based on the assumption that the particle transfers heat to the substrate by thermal conduction, by virtue of the temperature acquired during the process. Hertz's theories were considered to analyse the impact behaviour under a dynamic load to assess the deformation of the substrate while the energy absorbed for the deformation of the particle was evaluated considering the ideal deformation. For the sake of brevity, the full calculation of the formula describing those contributions is not here reported.

Knowing the deformation of the particle and its penetration into the substrate, it is hence possible to evaluate the impact velocity with the following formula (Eq. 1):

$$v = \sqrt{\frac{2}{m} \left(\frac{H_c(T_p - T_s)2s}{v_p} + \left(\frac{\pi a^{*4} p_d}{4R} \right) + \left(\frac{3}{4} \cdot Y_p \cdot V_s \cdot \ln \frac{r_0}{r_1} \right) - N\frac{f}{2}K_B T_p \right)} \quad (1)$$

With H_c thermal conductivity of the system, T_s substrate temperature, s space covered by the particle during the penetration, v_p is the velocity during penetration, a^* radius of the contact area at the point of maximum compression, p_d mean contact pressure during dynamic loading, R average radius of curvature in the contact area, Y_p yield stress of the particle material, V_s volume of a spherical particle, r mean radius of the particle and r_l is the semi-minor axis of the deformed particle. Those terms were calculated experimentally or were present in literature.

Finite Element Simulation of the process. 2D FE simulations of the impact and particle deformation were conducted using ABAQUS software to generate datasets. A Lagrangian algorithm was chosen as suggested by literature [24–26]. The particle diameter chosen for the simulation was 30 microns, accordingly with the mean particle size of the powder used for the experimental tests. The characteristics of both the substrate and the particles are present in the literature and obtained with previous tests on the materials available at the experimental facility.

The material behaviour of both the particle and the substrate was modelled according to the Johnson-Cook model for plastic materials and one of the algorithms available in ABAQUS software (surface-to-surface penalty contact algorithm) was used to model the contact process between the substrate and the impacting particle.

The model provided 40 values of penetration of the particle and flattening ratio varying the impact velocity.

Univariate linear regression. As this work is a preliminary outlook to theory-guided machine learning application to cold spray technique on polymeric materials, a univariate linear regression model is proposed in order to assess the feasibility of this approach. For this reason, a single parameter (feature) at a time have been considered.

Two different cases were evaluated:

- The estimation of the penetration depth known the impact velocity
- The estimation of the deformation of the particle knowing the impact velocity.

Upon the creation of datasets, the data was split into two parts: 70% of data were used for training while 30% for validation.

The hypothesis function chosen was a linear function reported in Eq. 2.

$$\hat{y} = h_{\theta}(x) = \theta_0 + \theta_1 x \quad (2)$$

Where \hat{y} is the predicted output vector, x is the feature vector and θ_0, θ_1 are the variables of the cost function (Squared error function [27], presented in Eq. 3)

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (\hat{y}_i - y_i)^2 = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x_i) - y_i)^2 \quad (3)$$

With \hat{y}_i predicted i^{th} value, y_i i^{th} actual output value and m number of training examples.

A gradient descent algorithm [28] was chosen to estimate the parameters in the hypothesis function (θ_0, θ_1) as in Eq.4:

$$\begin{aligned} \theta_0 &:= \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x_i) - y_i) \\ \theta_1 &:= \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (x_i (h_{\theta}(x_i) - y_i)) \end{aligned} \quad (4)$$

With α learning rate was set to 0.01. The gradient descent algorithm was repeated until convergence for a number of iterations of 450.

Before the training, the features were normalized in order to speed up the gradient descent using feature scaling and mean normalization $x := \frac{x - \mu}{s}$, where μ is the average of all the values for the feature, and s is the standard deviation of the feature x .

After the training, the maximum prediction error value and Root Mean Square Error were recorded and plotted. The Root Mean Square Error (RMSE) [29] was calculated with the following formula

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (\hat{y}_i - y_i)^2}{N}}$$

With N number of test data (in both cases 13 values were considered). The model code was written in C++ and executed in MATLAB.

Results and Discussion

For the first case considered, the impact velocity was chosen as a feature and the penetration depth as the output. Fifty training examples were fed to the model.

The surface and contour plot of cost function evaluated in theta values are portrayed in Fig.3.

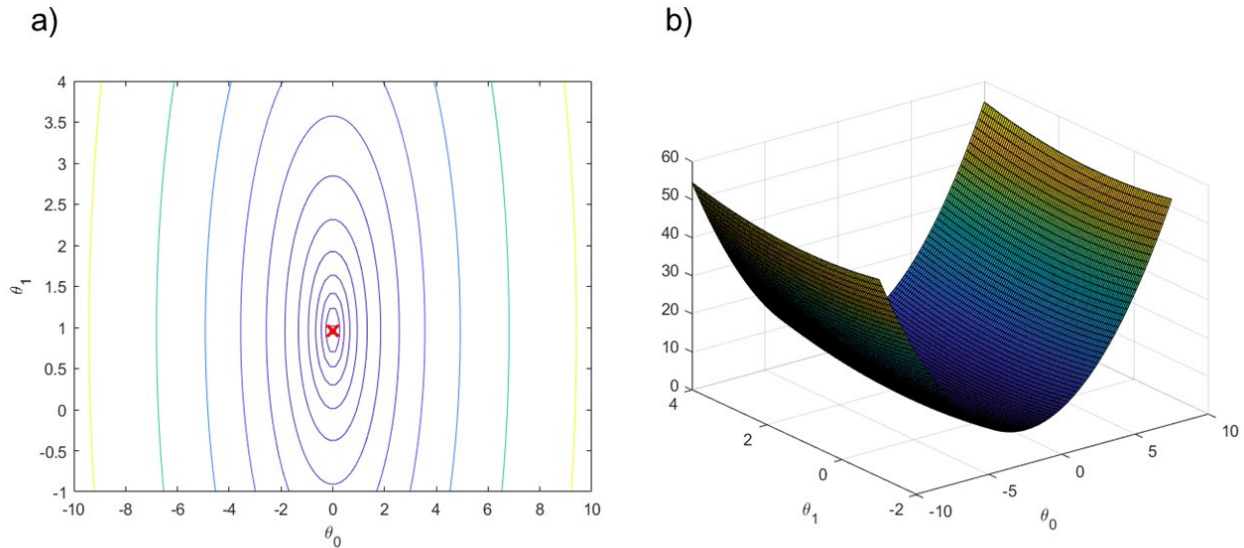


Fig. 3 - a) Contour plot of the cost function (J) varying θ_0 and θ_1 during the gradient descent iterations for the evaluation of the penetration depth known the impact velocity b) surface plot of the cost function (J) varying θ_0 and θ_1 during the gradient descent iterations for the evaluation of the penetration depth known the impact velocity

The theta values that guarantee the minimum of the cost function, estimated by the model after 450 iterations were:

$$\begin{aligned}\theta_0 &= 0 \\ \theta_1 &= 0,95\end{aligned}$$

Observing the previous figure, Fig.3, it is possible to assess that those values are very close to the minimum of the cost function. The hypothesis function was estimated as $h_{\theta}(x) = 0,95x$

As it is possible to observe in Fig.4, this function well follows the trend of the training example considered.

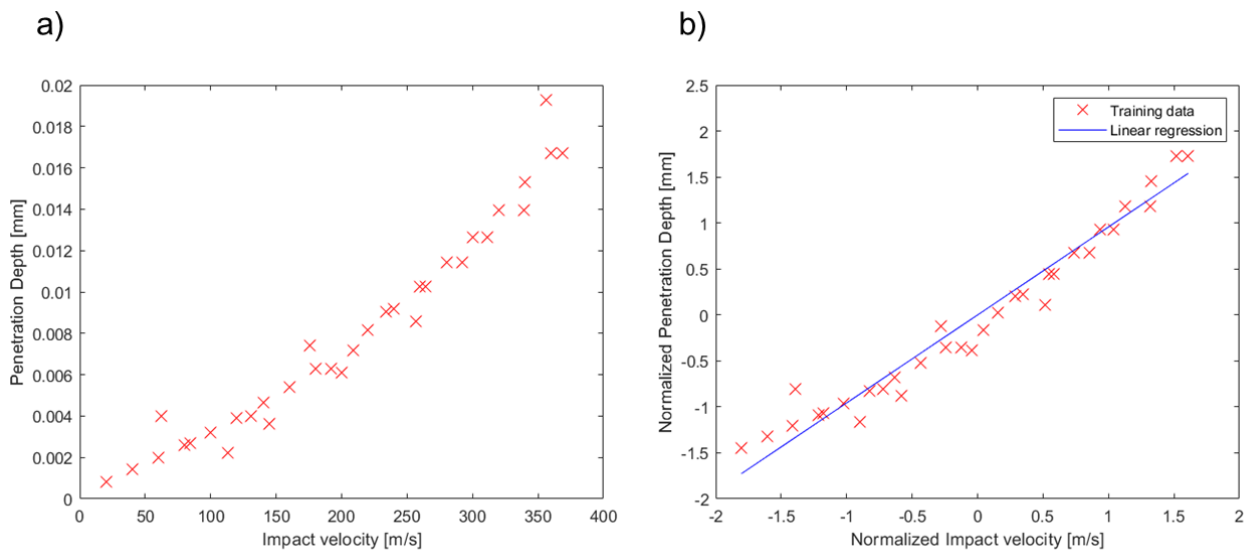


Fig. 4 – a) Plot of the training set values of penetration depth VS impact velocity b) hypothesis function plot for the evaluation of the penetration depth known the impact velocity

A non-linear function (as a quadratic equation or a square root equation) could provide better results and this will be further investigated in future works.

After the training, the Root Mean Square error was evaluated. In this case, the value of RMSE was $RMSE=0.2713$. As it is possible to assess observing Fig. 5 and analysing the RMSE value, the function obtained allows predicting accurately the test dataset values.

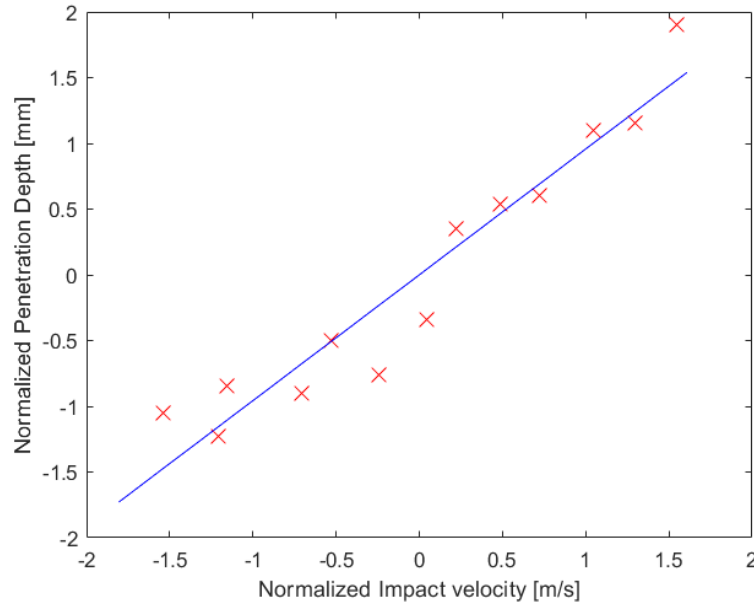


Fig. 5 – Plot of the normalized test set values of penetration depth VS impact velocity and hypothesis function

As regards the second case evaluated, the impact velocity was chosen as a feature as well but the deformation of the particle was chosen as the output. The number of training examples considered was fifty.

The surface and contour plot of cost function evaluated in theta values are shown in Fig.6.

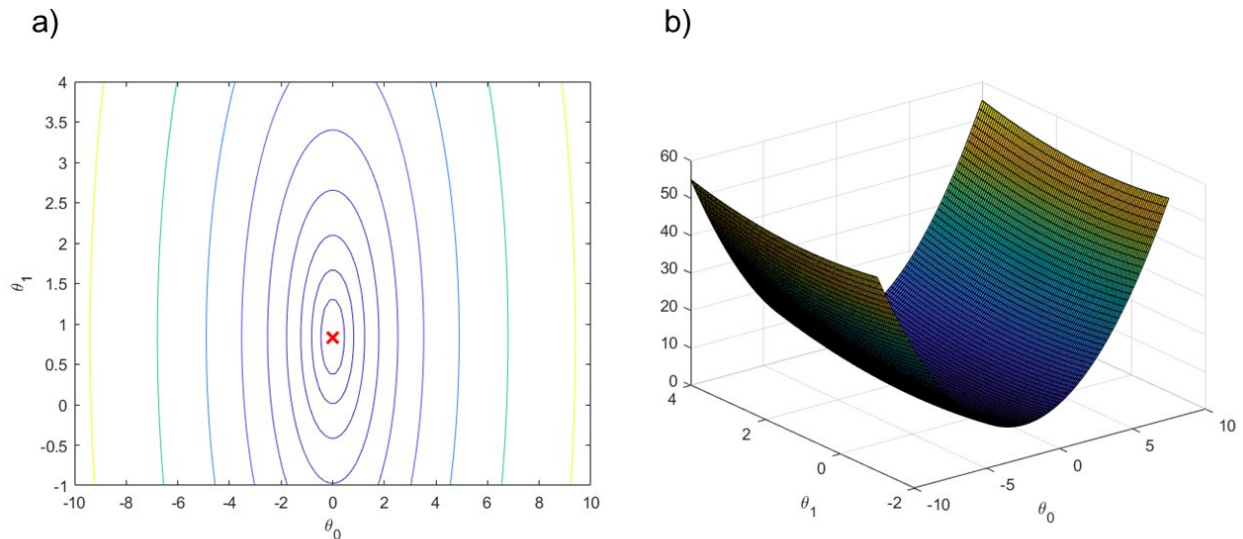


Fig. 6 - a) Contour plot of the cost function (J) varying θ_0 and θ_1 during the gradient descent iterations for the evaluation of the flattening of the particle known the impact velocity b) surface plot of the cost function (J) varying θ_0 and θ_1 during the gradient descent iterations for the evaluation of the flattening of the particle known the impact velocity

In this case, the theta values that ensure the minimum of the cost function, estimated by the model after 450 iterations were:

$$\begin{aligned}\theta_0 &= 0 \\ \theta_1 &= 0,83\end{aligned}$$

So it was possible to write the hypothesis function as $h_{\theta}(x) = 0,83x$. As in the previous case study, the contour and surface plots were obtained and portrayed in Fig.7.

Fig.7 show the data and the regression function obtained training the model.

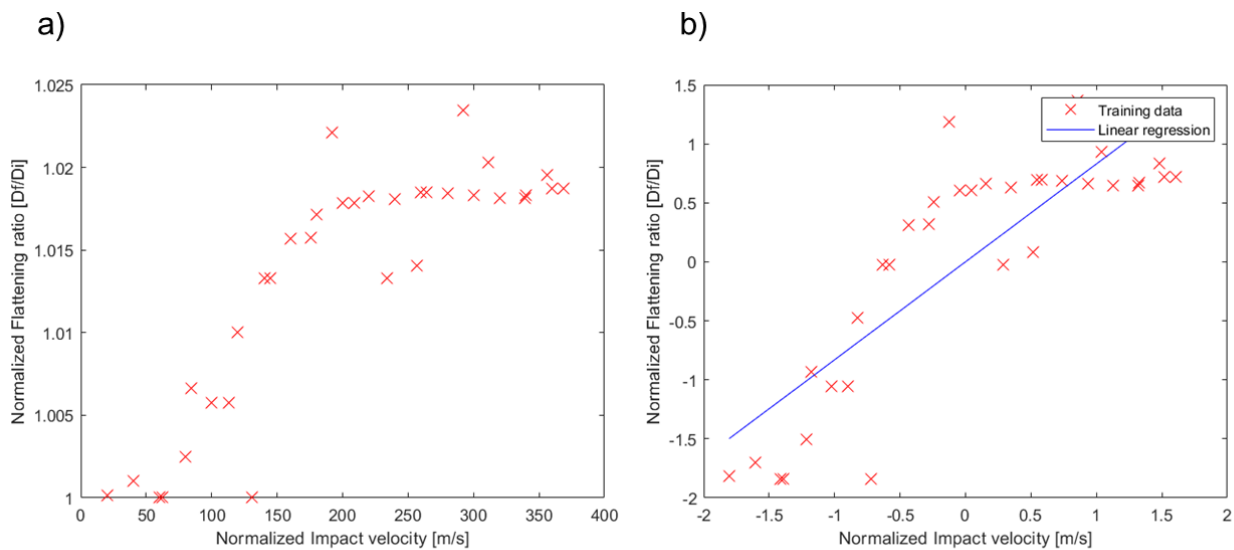


Fig. 7 – a) Plot of the training set values of flattening VS impact velocity b) hypothesis function plot for the evaluation of the flattening known the impact velocity

Due to the higher scatter portrayed by the training examples, the hypothesis function does not strictly follow the trend of the training examples, so the predictions provided by the model are much less accurate compared to the first case analyzed. For this reason, a cubic function would probably fit this case better than a linear function.

The RMSE was as well evaluated and the value obtained was $RMSE=1.0206$, noticeably higher than the previous case. As above hypothesized, a univariate linear regression is not suitable to model this case study, and this is furtherly confirmed by observing Fig.8.

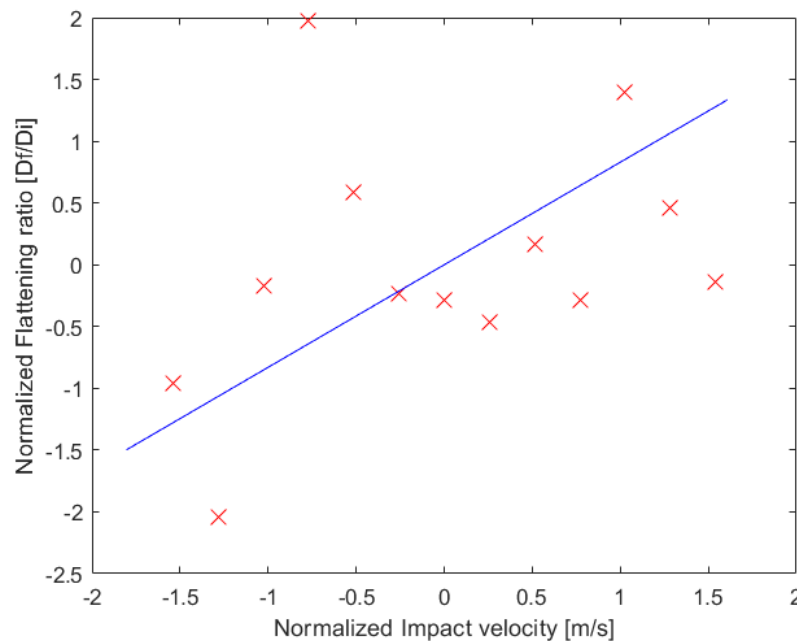


Fig. 8 – Plot of the normalized test set values of flattening VS impact velocity and hypothesis function

Conclusions

This work dealt with the possibility of using machine learning methodologies to optimize the cold spray process. In particular, this first investigation employs a univariate linear regression approach to predict the values of deformation and penetration of a single particle of copper impacting a peek substrate, knowing the impact velocity. The training set was composed of examples obtained using both a mathematical FE model and experimental results.

An analytical model was used in order to evaluate the impact velocity of the particle for the experimental samples.

The analysis confirms that this method could provide interesting results for the comprehension and optimization of the Cold Spray process.

Further analyses are necessary to improve the model presented. In particular, a non-linear model or a multivariate regression model could be considered in order to take into account the different parameters influencing the deposition and better follow the trend of the experimental results.

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