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State-of-the-art of numerical simulation of laser powder Directed Energy Deposition process

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Abstract

Additive manufacturing (AM) has been experiencing considerable growth in recent years, especially for metal application. Directed Energy Deposition (DED) is one of the emerging technologies in metal AM. DED selectively deposits material and melts it with a focused high-energy source. Accurate numerical modelling of the DED technique is an important step for the comprehension and the technological improvement of the process, providing significant gains in terms of time and costs. This paper aims to review the existing knowledge on DED numerical simulation, highlighting principal advantages and limitations of different approaches. The key inputs required to model the process properly, and the predictable outcomes are discussed.

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Keywords: Numerical simulation; Directed Energy Deposition; Additive manufacturing; Process modelling

1. Introduction

One of the latest advances in metal Additive Manufacturing (AM) is the Directed Energy Deposition (DED) process. Its applications are already numerous across many industries but, while other metal AM processes have been studied and tested for a long time, DED is a relatively *young technology*, so its potential has not been fully exploited yet. However, companies show great interest in its research and development, making this technology one of the new boundaries in industrial 3D printing. DED technology works by depositing the raw material while melting it on a surface, thus creating the melt pool that rapidly solidifies generating the track. DED machines are equipped with a deposition head, usually mounted on a multi axis arm, and the parts are created by the relative motion between the head and the build plate. The introduction of the multi axis arm allows the deposition of material in various directions and different angles: this complicates the understanding of the physical phenomena of the process but allows much more freedom to component design, elaborate geometries, and overall complexity. Moreover, the process can be classified by its energy source (laser, electron beam or electricity) and its

feedstock (powder or wire) [1]. The main advantages of this new technology are essentially the possibility to create larger parts compared to other metal AM technology, and the rapidity with which these parts are created. With this technology, functionally graded materials can now be created. Anyway, since now, DED process finds its main application in repairing: in fact, the way in which the process works allows to repair many components of various dimensions and materials [2]. Compared to conventional repairing techniques (such as welding processes), DED entails a smaller heated affected zone (HAZ), allowing to modify a smaller zone of the part.

Notwithstanding all the benefits described above, there are some disadvantages mainly related to the novelty of the process. In fact, the high-speed of the process can compromise the accuracy, in particular the superficial roughness. Also, the choice of process parameters affects greatly the porosity and the microstructure of the final components, which can result in poor part performances. The disadvantages are mainly related with the complex physical phenomena that occur during the process, such as solid-liquid transition, microstructure evolution, or laser/powder interaction. The research of a feasibility window for the process parameters is a key element to allow to build or

repair parts with good mechanical properties. The optimal process parameters can be found out in different ways: carrying out an extensive experimental campaign, (meaning a great cost in terms of money, materials, and time) or a numerical simulation of the process (which allows less expense).

This paper will focus on modelling and simulation of Directed Energy Deposition process, presenting the principal modelling techniques that are available in the literature, highlighting which are the main phenomena that each model aims to simulate, and the main advantages and the challenges still open in modelling approaches.

2. Numerical modelling for DED process

DED process is characterized by a variety of process parameters [3], as laser power, beam spot diameter, shielding gas flow, scanning speed, powder feed rate, powder and building platform material properties, scanning strategies etc. combined with many different physical phenomena as transient temperature and heat flow, rapid heating and cooling cycles, blown powder dynamics, laser/powder interaction, solidification phase, and complex transport mechanism (convection due to Marangoni effect, radiation followed by shielding gas and conduction of heat into the substrate) [4]. To fully understand the physics behind the process all the interaction among parameters and mechanism should be considered. However, considering all the interaction could lead to an impracticable and too complex model and usually the process is analysed as a sequence of steps, each one focalized on a specific phenomenon neglecting interaction among them. In fact, a variety of numerical models have been implemented for DED processes, but each model focuses on a specific aspect and thus provides limited appraisal of the overall part characteristic. Therefore, an integrated multi-scale model could be helpful to link the process parameters to resultant microstructure and mechanical properties to estimate the DED part quality comprehensively. Nevertheless, numerical simulation of the process is a fundamental tool for predicting the final characteristics of the produced component. Aiming to determine the correct range of variation of parameters, it is noted that the support of numerical modelling and simulation is fundamental to shorten times and costs compared to the experimental campaigns. Basically, applied to the DED process, numerical simulation allows to predict the temperature below the deposition surface, which is experimentally difficult. Residual stress and distortion, that lead to a loss of dimensional accuracy, result from the localized high heat input, characteristic of the process. Further, the microstructure is influenced by the DED thermal cycle with the rapid localized heating and cooling, but thanks to simulation tools microstructure growth and evolution during the process can be estimated. Experimentally instead, only the components' final microstructure can be observed. Even if numerical simulation process technique presents many advantages, it represents an approximation of the process and cannot prescind from experimental calibration and data validation. The simulation, ultimately, allows a swifter approach in finding the correct process parameters when in need to change inputs such as material, feedstock type or design adjustments.

The need to link the input parameters and the final output is greatly important. Numerical simulation also can help to understand which precise process parameter influences a specific final part characteristic, such as surface roughness, porosity, dimensional accuracy, and residual stress state. As seen above, the physical phenomena to be modelled are various and complicated and each of them occurs on a different scale of size [5,6]: macro-scale, meso-scale, and micro-scale. For this reason, several models have been developed over the years on various scales of size, both for input and output, such as the microstructure or final stress and deformations. Furthermore, the models can be weakly coupled or strongly coupled. In the first case, the various models are run separately, taking the output of one as the input of the other. In the second case they are performed together and influence each other throughout the process. Although the second method generates a better result, it requires a considerable computational cost, therefore, since even the first method can give good results, it is often chosen. Moreover, there are many similarities between the welding process and the DED process, such as the thermal cycle, the great thermal gradient, the solidification process. Weld numerical modelling has been an active area of studies for nearly four decades, in fact many modelling approaches that are used to simulate DED processes are based on previous research of the welding techniques [7-11]. Moreover, one of the main challenges in numerical simulation is managing a huge amount of data. In fact, DED process simulation reported difficulties in computing power and running time, especially when a massive component fabrication is simulated. High precision in modelling frequently correspond to high computational costs to the great amount of data to be managed. Therefore, a primary goal of various research is to find the right compromise between accuracy and computational costs. This goal is valuable also to AM industries which require efficient computational approaches that can be performed in affordable computational cost and time.

2.1. Macro-scale modelling approach

Simulations at macro-scale are mainly useful to predict the thermal-mechanical behaviour of DED components. Usually, these models are based on finite element analysis (FEA), and aim to predict temperature distribution, residual stress, and distortion [11-14]. Residual stress is one of the main drawbacks in DED process. Residual stresses can adversely influence mechanical properties of the components and can reduce the geometrical accuracy of the parts while affecting their final performances [12,15,16]. Residual stresses result from high thermal gradients and cooling rates, and these stresses persist in the material after the removal of the energy source leading to thermal distortion or even cracks [5]. Residual stress field is affected by many different process parameters such as scanning strategies, scanning speed, dwell time, laser power and build orientation, for these reasons many works focused their attention on the influence of process parameters on residual stress and distortion [12,17]. Moreover, the moving heat source causes a non-uniform high heat transfer leading to anisotropic inherent strains respect to the scanning path. Lu *et al.* [12] and Chen *et al.* [14] in their works analysed the effect of the

scanning strategy on distortion and residual stress in DED components. Lu *et al.* [12] analysed the effect of building strategy on the thermomechanical response of titanium alloy samples using a weakly coupled thermomechanical model implemented in Comet. After the model's calibration they were able to demonstrate that the vertical deviation can be significantly reduced by the scanning strategy, but the residual stress can be much more reduced by the preheating of the base plate. Instead, Chen *et al.* [14] proposed a continuous laser scanning path optimization that present the scalability to much taller and complex structures made up of multiple layers and features. They also pointed out that the scanning path and part design can be concurrently considered to minimize residual stress in metal AM components. Another approach, already used in Laser Powder Bed Fusion (L-PBF) application to enhance geometrical accuracy, is made by changing the geometry to compensate the distortion and lead to the desired shape of the part. Biegler *et al.* [18] used transient numerical simulation to obtain the compensated geometries for industrial-scale components. At first, a thermo-mechanical model was used to derive the parts' distortion, then results were inverted to derive the compensated geometry. They demonstrated that after a single compensation iteration, distortions can be reduced by over 65%. Moreover, Stender *et al.* [19] found out, by way of a finite element analysis workflow, that the higher value of plastic strain, residual stress and distortion are reached close to the baseplate and generally the peak in these values arise at the interface between successive layers. They validated their results on cylindrical samples built by LENS process.

Most of these FE models simplified the modelling of the material addition by considering the blown powder not conductive (inactive) until the powder reaches the melt state. Each element can diffuse energy by heat conduction when is classified as active in the model, and this is possible when the nodal temperature of the element has reached the melting temperature due to the application the laser energy [12,19-22]. To accurately model temperature distribution, residual stress, and distortion it is crucial first choose and calibrate the required properties of the heat input (as beam power and scanning speed), thermal boundary condition and material properties (as beam absorptivity, thermal conductivity, specific heat capacity etc.). In fact, a little variation in predicting the temperature evolution of the process has a great influence on the calculation of residual stress during thermo-mechanical simulation [9]. That revealed the importance of an accurate prediction of thermal behaviour in DED components. Khanafer *et al.* [22] proposed a finite element model implemented on Ansys to evaluate transient heat transfer process in DED parts. As other many authors [14,17,18], they represented the laser heat source as a Gaussian energy distribution. Further, Nijhuis *et al.* [23] presented a thermal model, but they tried to save calculation cost and time introducing a simplified heat input model basing it on prescribed temperatures. They were able to demonstrate that the hot element addition strategy can be efficiently used for thermal simulation of large-scale metal DED parts.

As it turns out, FE modelling has been widely applied for the prediction of thermal-mechanical behaviour of DED components. However, it becomes more expensive in terms of computational cost as the size of the modelled geometries gets

larger because these geometries require meshes with a greater number of nodes to be represented. Therefore, Li *et al.* [16] proposed a mesh coarsening strategy to predict temperature, distortion and residual stress. They compared two type of coarsening strategy with a static mesh type and found out that the computational time can be reduce by 75% with an error less than 2.5% for thin wall geometries built from Inconel 625 and Ti-6Al-4V samples. Other approaches have been used to save computational significance, Lu *et al.* [20] proposed a thermo-mechanical model to study the thermomechanical behaviour of more complex geometries of Ti-6Al-4V fabricated by DED process. They showed that the computational time can be reduced if a 4-layers-by-4-layers activation strategy is used, not affecting the average values of both temperature and distortion. Kiran *et al.* [9] were able to reduce the computational time both using a thermal cycle heat input and a lumping of layers strategy. The thermal cycle heat input consists in considering the complete deposition track as one block and reports the multiple steps of the transient heat input numerical calculation to a single step. Firstly, they validated this method on single tracks and multi-tracks and then transposed it to the construction of a cube, where the computational time required by the transient heat input is great. In the cube the entire layer was considered as one single block. To further decrease the computational time, they introduced the lumping of layers, meaning incorporating multiple layers in one single layer in the numerical model. They find out that the best numbers of lumped layers are two or four, that can reduce the computational time maintaining a good accuracy in results.

2.2. Meso-scale modelling approach

Meso-scale approach aims to simulate the fluid flow and the heat transfer in the molten pool that are the principal physical phenomena that determine the melt pool characteristics. Melt pool thermal and physical behaviour is greatly shaped by process parameter as laser power, powder feed rate and scanning velocity [24-28]. In particular Fatoba *et al.* [27] developed a model to obtain insights on the behaviour of melt pool subjected to various process parameters. The melt pool characterizes the deposition track geometry and topology that has an influence on the final characteristics of the DED components as residual stress and cracks. Instead, density and strength of components are more affected by the powder concentration. To simulate the fluid flow within the melt pool is necessary to include in the model the mass and momentum equation alongside the energy equation [1]. Wei *et al.* [26], also, directed their work on the effect of process parameters on liquid metal flow field and transient temperature of the melt pool. Especially they displayed that the contact angle of deposited single tracks increases with higher Mass per Unit Length intensity but decreases significantly with higher Energy per Unit Mass. The contact angle of the tracks can be a revealing parameter in predicting voids in the final parts when several single tracks are deposited next to each other.

Gas-powder flow distribution below the deposition head, instead, is usually modelled via Computational Fluid Dynamics (CFD) simulations [25]. CFD software works by a system of non-linear partial differential equations that describes the

motion of the fluid, diffusion, and phase change. Moreover, considering the Marangoni effect leads to great accuracies in the melt pool temperature distribution and geometry, but at the same time increases difficulties in computational calculation, Marangoni effect is related to the mass transfer along an interface due to the surface tension gradient. In fact, the main physical aspect that determines the fluid flow in the melt pool is the spatial variation in the surface tension on the melt pool surface. This spatial variation is caused by the great thermal gradient that can be controlled and adjusted by varying the feature of the energy source [29]. Zeng *et al.* [25] presented a CFD simulation to compute gas-powder flow behaviour coupled with a FEM analysis to evaluate thermal behaviour of the deposition track. CFD model gives as output the particle mass concentration, a key parameter to get the density of particles on a specific plane or volume. They found out that matching the laser beam focal point and the position of the highest particle mass concentration is fundamental for the full melting of the deposition inducing high-quality deposited tracks. On the other hand, Safdar *et al.* [30] in order to overcome computational burden of CFD models investigated the possibility to use the isotropic enhanced thermal conductivity models, to detail the melt pool convection. They revealed that these types of approaches cannot be very useful when applied on high Prandtl number materials like Nickel. So, they proposed and investigated the anisotropic enhanced thermal conductivity approach revealing that it can be much more appropriate and flexible for these types of materials.

Instead, Piscopo *et al.* [6] proposed an original method to model material addition and energy flow in order to evaluate geometrical characteristics of deposition tracks. In their model the effective power useful to heat up and melt both powder and the substrate was calculated as the sum of the power available at the substrate plus the power absorbed by the in-flight powder. This power can be expressed as a percentage of the total available power, and by means of experimental data they calibrated the value of the correction coefficient for the power. Moreover, the activation strategy applied in this work was based on analytical relationships derived from regression analysis that linked height and width of the deposited tracks to process parameters, namely laser power and the scanning speed. Through this model they were able to predict the deposited track size with an error lower than 8% and to evaluate the penetration depth of the tracks. Also, Vincent *et al.* [24] directed their attention on the geometries of the deposition tracks. They proposed a novel numerical simulation technique that can predict width and height of the deposition track relating them to the thermal gradients, fluid flow, melt pool shape and size. They combined a thermal fluid numerical solution with a geometrical model to consider the mass addition and an analytical model for the track geometry. They were able to find a balance to accuracy and computational cost by simplifying assumption about the behaviour of the gas-liquid interface.

2.3. Micro-scale modelling approach

Micro-scale modelling is typically a phase-field modelling used to predict the microstructure evolution during the deposition process. The study of the microstructure is of great

importance to understand the process and to obtain the desired mechanical characteristics of the part, such as porosity, density, strength etc. As well, microstructure evolution can give insight of the mechanisms that control defect formation in DED components. Therefore, it is essential to expand the knowledge in the microstructure formation and evolution mechanisms. There are three main microstructural modelling approaches: phase-field modelling (PFM), kinetic Monte Carlo (MC) and cellular automata (CA). Kinetic MC and CA modelling differ from PF modelling because they can only model the grain structure. Instead, PF models include modelling of solidified materials, solid state phase transformations, solidification segregation of alloys, grain structure, grain-oriented direction, grain coarsening etc. [5,31-33]. DED microstructure results from the rapid cooling, great thermal gradient typical of the process, and the ratio of cooling rate/thermal gradient [34]. Microstructure is also influenced by process parameters such as build direction, scanning speed, power beam etc. [35-38]. DED components mainly show columnar grains, equiaxed grains and a mix of columnar-equiaxed grains that consist of cellular dendrites [1,34,36]. This type of morphologies has been demonstrated to be mostly consequence of the temperature gradient at liquid/solid interface and the ratio of cooling rate-thermal gradient [36]. The growth of the grains follows the direction of the maximum thermal gradient i.e., the build direction, that creates an anisotropy in the component that implies a dependence on the type of scanning strategy of the components' mechanical properties [32].

To simulate components microstructure, is essential the temperature evolution experienced by parts, as it is required as input for microstructure models. This temperature evolution can be evaluated by experimental measurements or predicted by a model as well. Baykasoglu *et al.* [32] presented a thermal-microstructural model for Ti6Al4V titanium alloy that couples the heat transfer calculations with phase transformation kinetics. They used a Finite Element (FE) method implemented in Abaqus to evaluate the temperature distribution and verified it with experimental results. Further, they used the volumetric phase fraction to model the microstructure evolution of the solid-state Ti6Al4V titanium alloy. The microstructure model coupled the thermal FE model via a written subroutine. Then, they demonstrated that this is an efficient approach for the selection of the best process parameters, predicting the microstructure evolution and allowing to obtain the desired mechanical properties. On the other hand, Kumara *et al.* [33] used the temperature measurements made at the first deposited track level as input. They studied the evolution of the microstructure during laser metal powder Directed Energy Deposition Inconel 718 and subsequent heat treatment through the phase-field method. The process was simulated with Micress, a commercially available phase-field software based on the multi-phase-field approach. They also used the precipitation kinetic modelling through JMatPro software to generate the Time-Temperature-Transformation (TTT) diagrams and Continuous Cooling Transformation (CCT) diagrams to investigate the effect of local elemental segregation on the precipitation of different phases. They demonstrated that a combined approach using the phase field modelling and transformation kinetic modelling is a feasible

Table 1. Selected studies on modelling of different DED phenomena.

| Model scale | Characteristic outputs | Software | References |
|-------------|-------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|--------------------|
| Macro-scale | Prediction of temperature distribution, distortion, and residual stress | Abaqus, Comet, Netfabb Local Simulation, Simufact Welding, Sierra | [9,11-14,16,18-21] |
| | Prediction of thermal behaviour | Ansys, Matlab | [22-23] |
| Meso-scale | Prediction of temperature distribution, melt pool geometry, and depositions geometrical characteristics | Abaqus, OpenFOAM, Ansys, Comsol | [6,24,26-28,30] |
| | Prediction of temperature distribution, melt pool geometry, and gas-powder flow distribution | Abaqus | [25] |
| Micro-scale | Prediction of microstructural evolution, solutes evolution, and segregation | Micress, JMatPro, Abaqus | [32-33,39] |
| | Prediction of grains structure and morphology and the dynamic behaviour of melt pool and heat affected zone | Proprietary code | [40] |

way to predict and understand the microstructure formation during DED process of Ni-based superalloys and subsequent heat treatments. The theory shows the evolution in time and space of multiple phase-field functions that represent the spatial distribution and orientation of the grains.

The main advantage of PF modelling is that can simulate multiple phenomena and results are very accurate, but it is very expensive in terms of computational costs. Therefore, Liu and Shin [39] proposed an integrated 2D phase-field modelling with a 3D DED model and 3D CA model. The approach allows to simulate the high temperature solidification and low temperature solid state phase transformation for the Ti6Al4V DED process. This model can predict the elongated beta grains of columnar shape, which are typical of the process. They demonstrated the advantage of coupling the CA and PF models compared to only CA model in capturing the details of the grain structure or compared to only PF model in saving computational cost. Sunny *et al.* [40], alternatively proposed a dynamic KMC models, that had the goal to overcome the limitation of conventional KMC models. In fact, through this approach they can change the spatial domain of the melt pool and heat affected zone with time. This allows grain morphology prediction of larger DED components made by multi-layers deposition, in which melt pool and heat affected zone may have much more variation than in smaller parts.

3. Conclusion

Directed Energy Deposition process is an emerging technique that gives compelling advantages over conventional manufacturing processes by granting the fabrication of complex structure, repairing valuable components, producing functionally graded materials, and reducing material usage. However, due to its novelty and the complex physical phenomena typical of the process, its spread in AM industry is limited. Hence the need of comprehensive studies supported by the numerical simulations. However, each model and simulation technique anyway must face its own challenges. The major challenge in process simulation is to develop a model that can result in knowledge at overall scale of DED component and building process to apprise engineering decisions. Moreover, to be practical, the prediction model must be able to compute results in a reasonable amount of time and with reasonable computing power, maintaining sufficient accuracy

in results. The objective is to keep enough physics fidelity to trust the outcome of the simulations. In fact, another limit in speeding up models' outcome is the necessity of numerical calibration on experimental campaigns.

About macro-scale approaches computational challenges are related with the possibility to simulate large DED components, that enhance the data that need to be managed. Much research tried to overcome this problem by coarsening meshes far from the heat input and lumping multiple layers together, finding a balance between saving computational costs and maintaining accuracy in results. Moreover, a challenge for thermal model is describing accurately the temperature evolution through an accurate modelling of the heat source input. Most of the time heat input is modelled considering estimated power and absorptivity. Instead, CFD approaches found out their major challenge in the description of melt pool surface tension and its variation with temperature. These variations play a fundamental role in the shape and depth of melt pool, and their behaviour is very heavy to compute. In fact, usually these models are used to simulate only single melt track. Finally, also micro-scale approaches must cope some challenges. PF models can only simulate a small volume region (as a single grain or few grains), even with a great accuracy, and require more calculations respect to MC and CA modelling technique. On the other hand, MC and CA models are more suitable in simulating large volume, since they require less computational costs. However, they can only predict the shape and the size of the grains, in addition CA models can also predict the angle, but do not have the accuracy of PFM. Anyhow, all the modelling tools such as described here and reported in Table 1 can advance and apprise knowledge of conditions during DED process as well as final outcomes of the process. Each model is specific for a certain scale and aims to simulate a precise behaviour, hence the choice of models comes down to the research requirements.

Concluding, a future development could be the implementation of in-process monitoring with numerical modelling to realize a closed loop control and better the DED parts quality. The process parameters could be adjusted layer by layer according to the response of monitoring techniques that can reveal errors in the deposition process. This global mechanism could really reduce errors and uncertainty and enhance parts quality by increasing performances and reliability of the process.

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