Numerical simulation of multiple particle impact process during cold spray of the Ti-6Al-4V powder onto the Ti-6Al-4V substrate

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Abstract

The metal cold spray is an additive manufacturing technique with great potentials in bulk component production and restoration/repair. The metallic powders are accelerated to supersonic velocities (up to 1,000 m/s) by the carrier gas of high pressure and temperature through the convergent-divergent (de Laval) nozzle and impact on the substrate to achieve layer-wise material addition through deformation-induced bonding. One significant advantage of this technique is to keep the powder and substrate temperatures well below their melting points so that the initial physical and chemical properties of the materials can be retained. However, the component fabricated by this process suffers from relatively low interfacial bonding strength and high coating porosity. Therefore, process optimization through numerical simulation and experiment is much needed to study the interaction between the particles and substrate during impact. In the current project, we use Coupled Eulerian and Lagrangian (CEL) approach to simulate the multiple particle impact process during metal cold spray and predict the coating porosity. Python code was programmed to auto-generate 100 particles in the model with size-dependent individual temperature and speed to mimic the experiment condition, and the porosity can be directly obtained after the deposition using a sampling volume cube in the pile-up. This enables us to directly predict the porosity from the simulation and compare it with the experimental results, which provides an invaluable tool for the metal cold spray process simulation.

Keywords: Coupled Eulerian-Lagrangian (CEL); Multiple Particle Impact; Metal Cold Spray (MCS); Porosity; Ti-6Al-4V coating

1. Introduction

Metal Cold Spray (MCS) has been gaining increasing attention in recent years, due to its relatively low processing temperature and high deposition rate. The Rolls-Royce Corporate Lab at Nanyang Technological University (NTU) has setup the facility to develop MCS process for Ti alloys [1] and Ni alloys [2], and achieved desirable mechanical properties such as high bonding strength and low porosity [3,4]. However, the detailed understanding of the process mechanism has not been carried out. Therefore, numerical simulation is much needed for these upcoming research activities as it is the most cost-effective method for the process study.

There have been many publications reporting on the parametric studies of metal cold spray process with different simulation approaches [5-9], including Lagrangian [5], Eulerian [6], Adaptive Lagrangian Eulerian (ALE) [7], Coupled Eulerian-Lagrangian (CEL) [8] and Smooth Particle Hydrodynamics (SPH) [9]. Xie [10] compared these approaches for single particle impact simulations and concluded that CEL provides the most robust and accurate solution, as CEL analysis is especially advantageous for simulating the extreme deformation and jetting that might take place when particles collide with the substrate [11]. Traditional Lagrangian elements tend to experience issues with solution convergence due to high elemental distortion. The Eulerian meshes, on the other hand, do not deform throughout the simulation and let the material flows through the elements. Therefore, no bonding interface can be traced. On the contrary, Eulerian-Lagrangian contact allows for fluid-structure interactions with clear trace of material interfacial behaviour. Moreover, Xie [10] created a multiple particle impact model based on Face-Center-Cubic (FCC) particle arrangement model to estimate porosity rate and residual stresses. Due to the uniform particle sizes and arrangement, a quarter symmetry model was used in the CEL Abaqus impact simulation to reduce computational cost. Ghelichi et al. [12] also studied residual stresses for a cold spray coating using a CEL simulation on 100 randomly generated particles based on a Rosin-Rammler particle size distribution. Furthermore, analytical calculations were used to determine particle temperatures and velocities were assigned to individual particles in accordance to their sizes. However, it has been proven by Song et al. [13] that only with valid description of the interface behaviour and bonding mechanism, the residual stresses can be accurately obtained through simulation. Hence, for multiple particle impact simulation, without particle-substrate and particle-particle bonding behaviour, it is not possible to accurately obtain the residual stress profile, but only porosity values. Therefore, in this work, we attempt to create a 100 particle model for Abaqus CEL impact analysis, combining the advantages of both simulations conducted by Xie [10] and Ghelichi [12] to predict the porosity in the MCS coating. Details of the model setup can be found in the following section.

2. The CEL simulation framework

2.1. Eulerian Domain and particle modelling

The Eulerian domain was constructed in a cuboid shape to allow easy generation of uniform hexagonal meshes. A uniform grid mesh reduces the computational time required for the analysis. The

characteristic element dimension has an influence on the time increment taken within the explicit analysis. It was created by selecting the Eulerian type in the 'Create Part' tab and extruded as a solid. Ti-6AI-4V Eulerian material properties was assigned, with a defined linear $U_s - U_p$ Hugoniot equation of state (EOS) model [14] with plasticity. Coupled temperature-displacement Element type EC3D8RT was selected for conducting dynamic coupled thermal-stress analysis. Due to the selection of EC3D8RT element type, Eulerian outflow boundary conditions cannot be specified. The Eulerian domain must be large enough to contain all particles and also the deformed shape of the particle on impact with the substrate. If the domain is too small, material will start to flow out of the domain, exerting unwanted stresses on the walls of the Eulerian domain and the particles.

In order to provide a more accurate representation the actual cold spray process, particle sizes were randomly generated within the Eulerian domain following a Rosin-Rammler (R-R) particle size distribution model. The positions of the particles within the domain were also randomly allocated, individual particle's velocities and temperatures were prescribed based on the particle diameter. Stochastic R-R is often used approximate particle size distribution and is represented by the equation:

$$Y = 1 - e^{-\left(\frac{D}{\bar{d}}\right)^n} \quad (1)$$

Where Y is the mass fraction of the particles that are smaller than a given diameter (D), $\bar{d}$ is the R-R diameter and n is the R-R exponent.

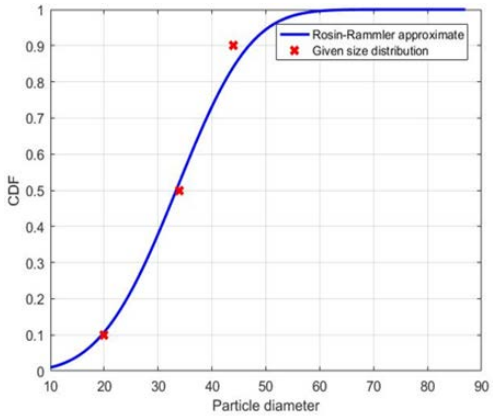

Fig. 1. Rosin-Rammler parameter approximation

R-R parameters ($\bar{d}$ & n) had to be determined based on AP&C's Ti-6Al-4V grade 5 powder with size distribution of 15-45µm [15]. The least-square fitting exercise was carried out as illustrated in Figure 1 and it obtains the approximated R-R distribution curve parameter $\bar{d} = 36\mu m$ and n = 3.533. The particle sizes were then randomly generated by using these parameters, uniformly sampling mass fraction Y and rearranging Equation 1 above.

The velocity of the particle impacting the substrate has a significant influence on the bonding formation. Larger particle diameters will have lower particle velocities, due to their higher inertia. Considering this effect, velocities can be approximated using the equation prescribed in the previous literature [16] and implemented in the current python script. Attempt to correlate the particle's temperature (T_p) and diameter (D_p) was made using a 3rd order polynomial and curve fitted to meet the results generated by computational fluid dynamic (CFD) analysis conducted by Arvinth [17], which was already validated by the experimental result in that work.

The particles were generated within a cylindrical domain specified within the user interface tab when running the python script. The coordinates [x,y,z] of the centre point within the spherical coordinates were chosen randomly. Initially, a position is randomly selected in the 2D (X-Y) polar coordinates and converted into Cartesian coordinates. Subsequently, the z coordinate was assigned randomly in the same manner. After the center position and radius of the particle have been fixed, Effective Volume Fraction (EVF) must be assigned within the Eulerian domain to represent each particle. The current particle part serves as a template to define discrete fields using the volume fraction tool. Elements within the particle will have EVF of 1, while elements at the particle's boundary will be partially filled (0<EVF<1) depending on the volume fraction the reference part occupies within the Eulerian element. The remaining elements will be void, meaning EVF of 0. Discrete field will be created for each particle. Subsequently, the Ti64 Eulerian material was assigned to all particle's discrete fields as a predefined field.

2.2. Lagrangian domain and model assembly

The substrate was modelled as a cylindrical Lagrangian domain as it does not experience very large deformations. The densest mesh can be found in the particle impact region, corresponding to the cross section dimensions of the Eulerian domain. It provides the required resolution to analyse the deformation on the substrate. The mesh size of the particle impact region should be close to the mesh size of the Eulerian domain to prevent material leakage into the Lagrangian domain. The Lagrangian C3D8RT element type was selected, which allows multiple materials, supports Eulerian transport phase and temperature advection. As shown in Figure 2, the Lagrangian substrate (in grey) occupies some region of the Eulerian domain (in red), pushing out any material within the Eulerian domain, turning it into void. This is to ensure that particle deformation will not cause material leakage out of the Eulerian domain.

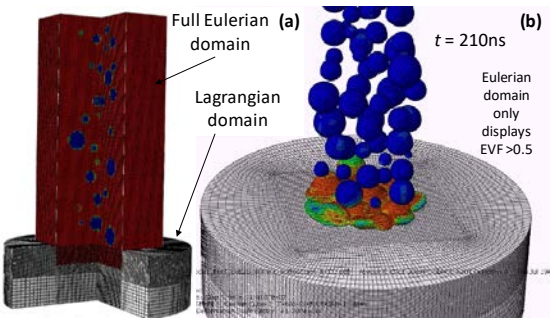

Figure 2: Model (a) assembly and (b) snapshot at time frame *t* = 210ns with Eulerian domain display EVF>0.5 only

2.3. Interface properties and analysis step

For the interfacial contact behaviour and bonding, a tabular pressure-overclosure relationship that

defined the interface normal behaviour can be implemented based on the authors' previous work [18], which was validated by single particle impact simulations and residual stress measurements. The tangential behaviour was trickier to prescribe, as there is no defined contact surface between the different particles within the Eulerian domain. The Eulerian particles tends to behave similar to droplets of fluid puddling, splashing, sliding and spreading across the surface without achieving significant coating thickness when no contact friction is prescribed. These 'splashes' or jetting might result in convergence error within the explicit analysis as the rate of deformation exceeds the wave speed within some Eulerian elements. A simplified way of tackling the above problem was to define friction coefficient (μ_k), forcing the particles to behave like a viscous fluid, providing some resistance to sliding and allowing the thickness of the coating to grow. Figure 3 shows the influence of friction on the shape and form of the deposited particles. It is clear that the presence of friction reduces the spread and increase the layer thickness, providing a better representation when compared with experimental results. It was determined a $\mu_k = 0.8$ provided the best match with experimental results. However, a more accurate way of prescribing the tangential behaviour of the particles as they bond with one another is needed. Perhaps by relating the amount of friction with the amount of shear stress between the surfaces of the particles as they impact one another.

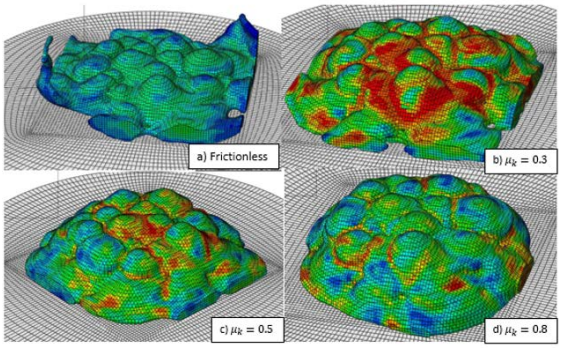

Figure 3: Influence of friction on one hundred particles cold spray deposition process simulation (a) $\mu_k = 0$ (b) $\mu_k = 0.3$ (c) $\mu_k = 0.5$ (d) $\mu_k = 0.8$

A pinned boundary condition was enforced on the bottom surface of the substrate to prevent any movement of the substrate as the particles impact. As conventional Eulerian boundary outflow conditions are not available due to the element type that was chosen, a potential future improvement would be to implement periodic boundary conditions for the outer walls of the Eulerian domain. Other than the predefined fields that were prescribed to the particles within the particle generation python code, the substrate must also be assigned a temperature. This was easily done by selecting all the nodes within the substrate and defining a fixed initial temperature of 373K (approximately 100°c). Other temperatures of the substrate can also be tested to investigate its influence to the process.

A coupled temperature-displacement dynamics step was assigned to model the particle impact. A time period was assigned from the initiation of the simulation till all particles' velocities are zero, depending on the model setup. It was set at a range of 700 ns to 1000 ns in the python code. Fields outputs such as EVF are selected for analysing porosity within the coating.

3. Results and Discussions

3.1. mesh convergence study

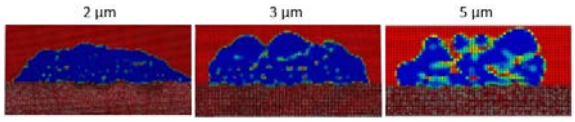

Figure 4: Cross sections of the deposition at different Eulerian mesh sizes

A porosity cuboid of dimension 120 x 120 x 20 µm was sectioned approximately from the middle of the coating elements to be used for EVF void calculation. The accuracy of this porosity calculation for each unique set of parameters would largely depend on the resolution of the mesh. The finer the mesh, the better small void regions are captured. By observing the results of simulations run at different mesh sizes of 1.5 µm, 2 µm, 3 µm and 5 µm, it could be understood that a finer mesh allows material to flow in a less viscous manner than a coarser mesh, as depicted in Figure 4. As a result, a finer mesh results in lower porosity as shown in the monotonic curve plotted in the Figure 5. Although a finer mesh produces results closer to the reality, one has to take into consideration the significantly longer computation time that is required in running simulations at mesh size 1.5 µm. Hence, for a better balance between accuracy and computation time, the optimal mesh size is suggested to be 2 µm.

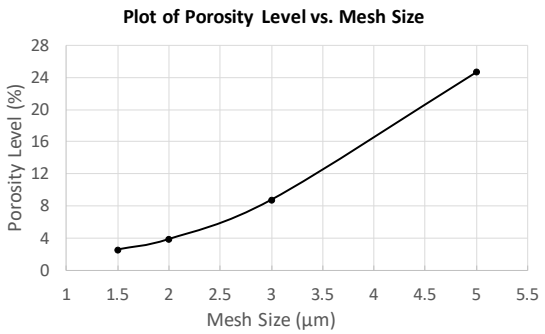

Figure 5. Porosity level with increasing Eulerian mesh size

3.2. model validation

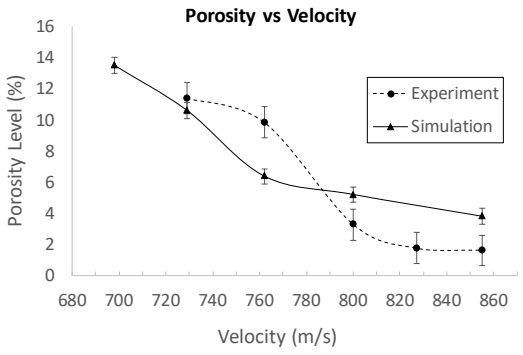

Figure 6. Coating porosity vs. particle velocity from experiment and simulation results

In the simulation, it was clear that the main factors that affect the porosity level of the coating are the particle velocity and particle temperature. The particle velocity could be manipulated by varying the gas temperature. Whereas, the changing of particle temperature is accompanied by varying the last constant in the particle temperature equation described in the python script. By adjusting the particle velocity and particle temperature to be close to the experiment's conditions, the porosity trend from the simulation can be obtained, and it aligns well to the experimental results, as shown in Figure 6.

3.3. Influence on the substrate temperature

During the experiment, the substrate was preheated to an elevated temperature for the aim of reducing residual stress and improving bonding strength. During the project, it was speculated that particle impact on the substrate may play a part in elevating the substrate temperature. To find out this, temperature profiles were extracted from the substrate. It can be observed that the particle impact does not heat up the bulk substrate, with heated zone less than 5µm in depth as shown in Figure 7. The thermal effect of the particle impact is proven to be very limited to the surface of the substrate and it can be quickly dissipated through thermal conductance. Therefore, the substrate temperature can be considered constant throughout the cold spray process. By assigning different initial temperature to the substrate, the effect of substrate temperature on the coating porosity can be investigated. Simulations were run with substrate temperatures at 373K and 473K to compare the resultant porosity levels, and both models yield a porosity value around 3.9%, indicating substrate temperature change does not affect the coating porosity level significantly.

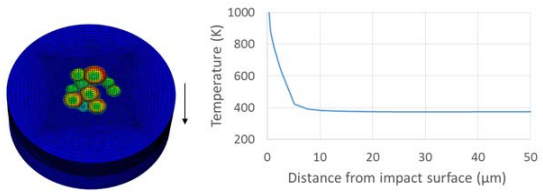

Figure 7. Plot of the nodal temperature vs depth in the substrate under multiple particle impact

4. Conclusions

In this work, a hundred-particles Abaqus model for CEL simulation of MCS process was created with an in-house python script. The particles sizes were randomly defined, following a predefined R-R distribution according to the manufacturer's specification. Each particle's initial velocity and temperature were automatically assigned based on its diameter, the gas temperature and Tp constant. Preliminary trials provided promising results which can be used to determine the porosity within the coating, and it is validated by the experimental results. Future work could be done to further refine the model in the area of adding tangential behaviour model for the interfacial bonding behaviour and implementing periodic boundary condition on the walls of the Eulerian domain to eliminate element boundary effects and potentially reduce computational time.

Acknowledgements

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