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Flow Visualization and Parameter Suitability in Cold Spray Titanium Deposition: A CFD Approach

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Abstract. Cold Spray is an emerging technology in the domain of additive manufacturing. It is a solid-state high strain rate material deposition technique. It uses a supersonic (2-4 Mach) impact of process gas (such as nitrogen or helium) to deposit micron-sized (1-100 µm) metallic or composite powder particles onto a substrate via a severe plastic deformation mechanism without any significant fusion. To have a successful deposition, the specific powder particles should travel above a material-dependent threshold velocity, which is called the critical velocity. The convergent-divergent nozzle is employed for achieving high velocities. The main objective of the current research is to study the flow visualization of two-phase titanium particle laden nitrogen gas in a simulated 2-D axisymmetric nozzle where particles are having a particle size of 25 microns, and to investigate the suitability of a specific set of cold spraying process parameters for the successful deposition of titanium powder using computational fluid dynamics. For the analysis, a two-equation realizable k-ε simulation viscous model was preferred due to its more realistic consideration of the cold spray process and reduced computational cost. Titanium powder particles will be successfully deposited using cold spray when operated at the precise set of process conditions on account of the average particle velocity observed at standoff distance higher than the critical velocity.

Keywords. Cold spray, Coating, Critical velocity, Viscous model, Computational fluid dynamics.

1. Introduction

Cold spray has emerged as a high production rate process for both surface engineering and additive manufacturing. In this technique, micron-sized powder particles are deposited by impacting them with supersonic velocities onto a target substrate material. When these high kinetic energy particles strike on the substrate, they undergo significant plastic deformation and stick on the substrate as a coating. The feedstock particles are accelerated by an expanding gas in a supersonic de-Laval nozzle. In this process, the temperature of the particle is well below the recrystallisation temperature, therefore the name cold spray is given to this process. Since temperature is low, deposits with high purity can be manufactured by this process. In contrast to other thermal spray techniques including high-velocity oxy-fuel (HVOF), plasma spray, and detonation-gun, this process is solid-state, therefore there is little oxidation and other compositional degradation of the sprayed powder [1]. A broad range of metals, including Cu, Al, Ti, Fe- and Ni-based alloys, as well as ceramics and cermets, can be deposited on a wide

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variety of substrate materials. As the deleterious effects of thermal distortions and heat affected zones (HAZ) are very minimal, it is a very reliable technology for coating temperature-sensitive materials such as amorphous and nanomaterials, and different powder material combinations with varied differences in their melting point temperatures [2, 3, 4].

The powder particle velocity at the exit of the nozzle immediately before hitting the substrate is a paramount characteristic in the cold spray method. The velocity should be above a threshold limit which is termed as critical velocity. All the powder particles crossing this material-dependent critical velocity will end up in successful deposition on the target substrate. If a particle's velocity is lesser than the critical velocity then either the powder particle will bounce off the substrate or it will impinge on the substrate leading to erosion of the same in case the velocity is higher than the erosion velocity [5-6].

Li et al. [7] performed numerical investigation of the cold spray procedure including the introduction of under- and over-expanded jets. By examining nozzle exit circumstances, they suggested a normal shock wave model to calculate the impact speed of powder particles in cold spray. In order to recreate the flow of gas phase and discrete particle paths in a supersonic nozzle both before and after colliding the intended target surface, Karimi et al. [8] effectively created the computational fluid dynamics framework of the cold spraying process. A recently published three-dimensional CFD simulation model for the cold spray process was developed by Zahiri et al. [9] and uses a two equation k-ε turbulence model. In this study, the model estimation was verified against experimental data by evaluating simulation findings. The titanium substrate temperature measured during the experiment was primarily used to calibrate the 3D model. The study found that the cold spray gas velocity and pressure predictions made by the 3D model were satisfactorily similar to the experimental data.

The present study introduces a computational fluid dynamics model that provides valuable insights into the flow visualization of nitrogen gas carrying titanium powder during the cold spray process. This model enables a comprehensive understanding and analysis of particle trajectories and the dynamic gas flow field within a convergent-divergent nozzle. Furthermore, it offers the opportunity to examine particle behavior in the proximity of the nozzle exit, both prior to and following collision with the target substrate plate. Moreover, the study conducts an investigation into specific process parameters to assess their suitability for achieving successful deposition of discrete titanium particles using the cold spray technique. Overall, this study offers useful information for optimizing the cold spray process in order to perform efficient titanium powder deposition.

2. Methodology for Computation Fluid Dynamics Analysis

2.1 Computational Domain, Meshing and Boundary Conditions

A specific de-Laval nozzle geometry has been considered for the analysis, which is being used in the cold spray system. The nozzle has a circular cross-section with a main gas pressure inlet diameter of 19 mm, pressure outlet diameter of 7 mm and throat of 3 mm. The nozzle barrel length is 15 mm with convergent and divergent section length of 55 mm and 175 mm respectively. The powder injection length is 30 mm with a carrier gas pressure inlet diameter of 2.5 mm. The substrate wall is at a standoff distance of 25 mm from the nozzle exit and has a length of 47 mm as shown in Fig.1.

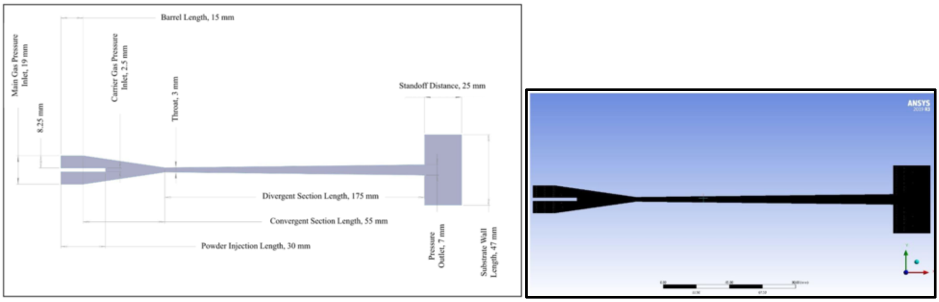

Fig.1 Computational domain and meshing of the cold spray nozzle.

The boundary limits applied in the 2-D computation domain and meshing have also been illustrated in Fig.1. The temperature and pressure of the main gas were set at a value of 873 K and 3 MPa while for the inner powder injection tube, a carrier gas temperature of 300 K and pressure of 3.1 MPa were applied. The titanium powder particles were considered to be spherical with an average diameter of 25 µm. The injection wall and nozzle surfaces were handled as viscous adiabatic. The ambient temperature and pressure were applied to each of the five boundaries that are exterior to the nozzle.

The nitrogen gas was permitted to flow in any direction at the substrate wall surface. The boundary limit conditions so applied prompted computed mass flow rates of N_2 of 1.35e-2 kg/s from the main gas annulus while 3.9e-3 kg/s through the powder injection inner tube. Titanium discrete powder phase is predicted to flow through the inner tube at a mass flow rate of 4.8e-4 kg/s. The detail of the discrete phase injection properties and gas particulars have been tabulated in Table.1.

Table.1 Detail of discrete phase injection properties (left) and nitrogen gas used as main and carrier gas (right).

Discrete Phase Injection Properties	
Injection Type	Surface
Injection Surface	Carrier Gas Pressure Inlet
Injection Direction	Normal to Surface
Particle Type	Inert
Particle Material	Titanium
Particle Material Density (kg/m^3)	4850
Particle Material Specific Heat (J/kg-K)	544.25
Particle Diameter (microns)	25
Particle Temperature Inlet (K)	300
Particle Velocity Inlet (m/s)	0
Particle Flow Rate (kg/s)	4.8e-4

Gas Details	
Gas	Nitrogen
Density (kg/m^3)	1.138
Specific Heat (J/kg-K)	1040.67
Thermal Conductivity (W/m-K)	0.0242
Viscosity (kg/m-s)	Sutherland

The implicit formulation was used as the converged steady state solution can be obtained easily on account of its broader stability characteristics when compared with explicit formulation. Initially, during the startup the value of the courant number was kept default (which is 5). The ROE-FDS (approximate riemann solver) flux type was employed since the boundary needed to be captured because of the discontinuity present near the boundary (like in shocks). The required convergence as per the residual absolute criteria was achieved after 10232 iterations.

3. Results and Discussions

3.1 Continuum Gas Phase Contour Maps

The velocity contour map for the nitrogen gas is depicted in Fig.2 (a), which clearly shows rise in the velocity along the nozzle's length. The velocity contour demonstrates that the flow from the de-Laval nozzle is supersonic and compressible. By transforming the pressure head (as evident from Fig.3) into a supersonic jet, the nozzle could achieve higher exit velocity. The maximum velocity of the gas phase at the standoff distance (SoD) is 1800 m/s which in turn corresponds to a Mach number of 3.5. Shockwaves develop when a supersonic flow adapts to disturbances (perturbations) or conditions downstream. In this particular case, it is the substrate which is creating the flow perturbations. Infinitesimal pressure waves are generated in the near vicinity on account of change in the momentum and molecular energy of the carrier gas. These pressure waves advancing at the speed of sound merge immediately ahead of the flow to form a typical shockwave as they are unable to move upstream or alert the flow to the presence of the substrate. The shockwave is separated and curving as shown in Fig.2 (b), this phenomenon is known as the bow shock. A zone containing a recirculating, minimal-velocity fluid experiences significant fluctuations and sudden shifts in the local flow characteristics within the confines of the bow shock. Within such a shockwave, the value of the velocity begins to decrease, whilst the gas density increases almost instantly. The dimensions of the bow shock are greater at much lower SoDs, resulting in a greater negative impact on the entrained particle velocity. Although the Cold Spray community has conducted extensive research on the nozzle SoD, there is no general agreement regarding its effects. Due to viscous effects, shockwaves and ambient mixing, the gas jet's velocity away from the nozzle decreases as SoD increases [4, 10]. Hence, an optimum SoD has to be chosen by taking these two competing mechanisms into account which are: the gas jet which causes particle acceleration/deceleration, and the bow shock promoting particle deceleration.

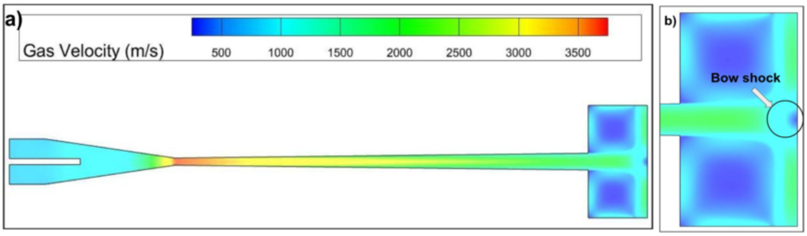

Fig.2 (a) Gas velocity contour map with nitrogen as the process gas at 3 MPa main gas pressure and 3.1 MPa carrier gas pressure (**b)** enlarged view closer to the substrate showing bow shock phenomenon.

The gas temperature contours are illustrated in Fig.4, with the main gas entering the de-Laval nozzle at a temperature of 873 K and carrier gas at a temperature of 300 K. The wall temperature of the nozzle after the throat is high because of the no slip phenomenon. Hence, the cooling is done through the coolant circulating inside the nozzle sleeve.

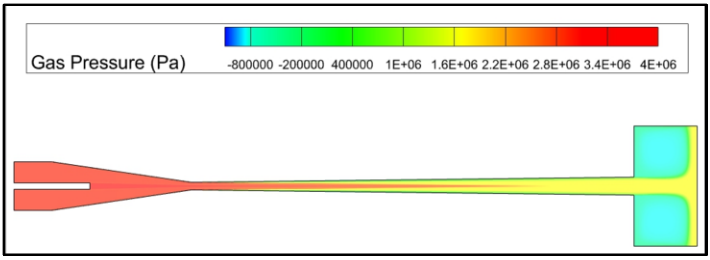

Fig.3 Gas pressure contours with nitrogen as the process gas at 3 MPa main gas pressure and 3.1 MPa carrier gas pressure.

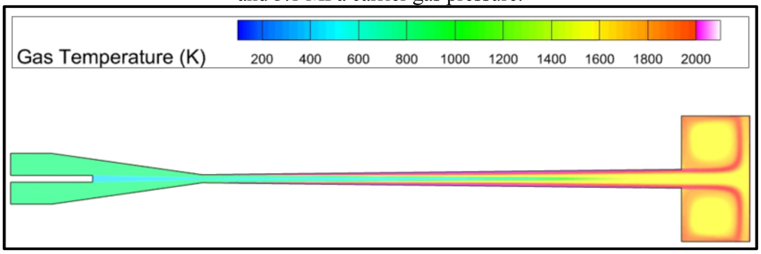

Fig.4 Gas temperature contours with nitrogen as the process gas at main gas temperature of 873 K and carrier gas temperature of 300 K.

3.2 Discrete Phase Contour Maps

The velocity contour map for the discrete titanium powder phase has been illustrated in Fig.5. According to Schmidt et al. [11], the critical velocity for the successful deposition of titanium powder particles having 25 µm size lies between 700 and 900 m/sec. The average particle velocity of the discrete phase at the SoD of 25 mm is coming out to be 946.2 m/sec, which is greater than the abovementioned critical velocity. This would suggest that the deposition is possible for this particular set of cold spray process parameters.

The temperature contour map for the discrete phase is displayed as shown in Fig.6. The average particle temperature is coming out to be 294 K, which is considerably lower than the melting point of titanium (1941 K). Hence, no compositional changes are expected in the discrete phase indicating an oxide-free deposition. Also, since the micron sized titanium powder particles are pyrophoric, thermal degradation at high temperature is possible, however this will be avoided in the evaluated temperature range (294K). It may be concluded that the intended (chosen) set of process parameters is capable of depositing the titanium powder particles in an efficient manner in solid-state, as per the mandate of cold spray.

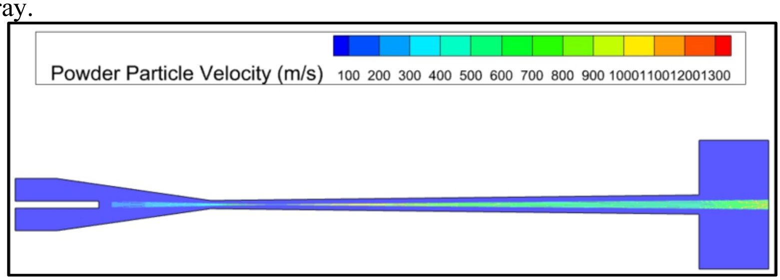

Fig.5 Velocity contours of discrete titanium powder phase.

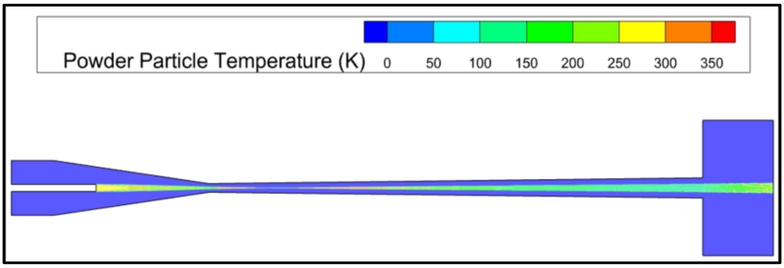

Fig.6 Temperature contours of discrete titanium powder phase.

Conclusions

- The cold spray process was successfully modeled using computational fluid dynamics for flow visualization of nitrogen gas containing titanium powder.
- The bow shock made at the zone of impact could be anticipated by the model, which is critical to comprehend since it lessens the speed of both the gas and entrained particles.
- The study shows that the standoff distance (SoD) needs to be optimized, because at lower SoD the size of the bow shock is more. It has a greater negative effect on velocities of discrete powder phase and process gas.
- The average particle velocity obtained at the substrate wall was greater than the critical velocity of titanium powder particles having size of 25 µm. Also, the average particle temperature was substantially less than the melting point which implies that the solid state deposition is taking place without any compositional changes in the powder feedstock.
- The intended set of cold spray process parameters was found to be appropriate for the successful deposition of the titanium powder particles.

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