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The Influence of Particle Flux Density and Particle Size Distribution in Surface Morphology of Cold Spray Coatings

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Abstract. In this article the coupling between the Cold Gas Dynamic Spray (CS) particle flight instance just before impact and resulting surface morphology after impact of a cluster of particles are investigated with a view to understanding the complex CS process for possible optimisation for the CS fabrication process in nano thin films. This study identifies two main variables for the analysis namely particle flux density and particle size distribution and examine their influence in the structural properties of the coatings, in particular, the deposition efficiency of the cluster of particles and its applications in functional properties of the coatings. This process determines the deposition parameters that characterize the surface roughness. Given r as a radial distance from the axis of a nozzle, and R as the maximum radial distance reached by the particles, the results indicate that increasing the flux density of a cluster beyond a certain limit (yet to be identified) creates a deformation behaviour closely related to that of a single particle, however this process lowers the deposition efficiency as r approaches R; where R is the radius of the nozzle particle flux distribution radius at impact surface and r is measured from the centre axis , (where $r = 0$), of the impinging particle jet to towards the peripheral (where $r = R$). A similar characteristic on the morphology of the surfaces is observed when particles have a varying particle size: the smaller particles (and indeed any other particle sizes) that hit the target substrate at the peripheral at an angular velocity and possibly with reduced velocity from the average particle flux jet velocity, eject outward due to the oblique impact imposed by the traverse velocity component. These findings have potential applications in fabrication of functional surfaces for various applications and provide us with control variables necessary for modifying the surfaces.

1. Introduction

The cold gas dynamic spray technology involves acceleration of particles to supersonic velocities (such as 400 – 1200m/s) for deposition in the manufacturing of thin films. The thin films so fabricated can be used for various applications; in our research we are more interested in applying this technology in nano thin films where the physical structure such as surface roughness and the material properties define device functionality [1].

Numerical methods assist in understanding the behavior of complex dynamical processes such as the CGDS process to variation in process variables. There are two main aspects involved in the systems analysis of a CGDS process: the fluid dynamics aspect [2, 3] which involve particle flight through the nozzles and outside the nozzle; and the solid mechanics aspect [4, 5] which involve the interaction of the particles and the substrate at impact (i. e the impact process). From a systems engineering aspect these two ends are coupled in the flight dynamics of the particles outside the nozzle, this involve the trajectories taken by the particles, the preferred trajectories for varying sizes; the preferred temperatures for varying particle size; the densities of the particles, and the preferred velocities for varying particle sizes. High pressure in the impact zone creates a bow shock which can deflect smaller size particles [6]. Further particles falling an appreciable distance away from the nozzle axis will be subjected to unbalanced traverse forces due to reduced pressure of axis which will give a traversal velocity component during their flight to impaction with underlying substrate material. Upon impact, depending on the adhesive or cohesive forces bonding or ejection of the particle will occur.

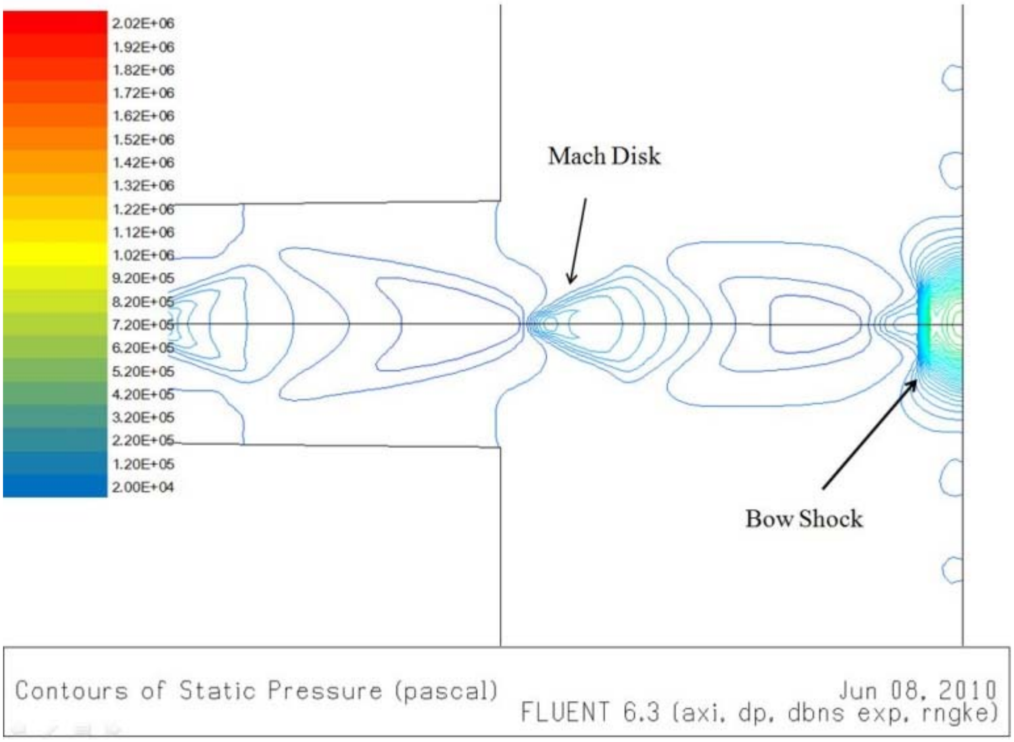


Figure 1. Pressure contour of N_2 outside the nozzle [6], bow shocks in high pressure CS systems.

2. Comparisons between modeling the cold spray process and practical applications of the CGDS

This study involves a numerical analysis of the impact process, and therefore the computational model begins with a capture of the particle instance just before impact of the first particle (see figure 2). As is the case in most numerical studies, this instance is normally simplified. In some instances, this is necessary in order to reduce the complexity of the problem setup. This simplification must be properly recorded as limitations of the computational model have effect of the extent to which the results will compare with practical applications. Usually it is acceptable to make these assumptions, and a comparison to any experimental data must discuss the variables involved in the experiments in comparison to those captured by the numerical methods. Sometimes the computational model may turn out to be more theoretical than is practical while in other instances the assumptions and simple models will be beneficial in determining the contribution of specific variables to the complex process under study. This process is illustrated in the block diagram of figure 2 where experimental results in [7] and numerical results in [4] are examined.

Due to limitations in numerical models, it is important to specify the limitations of the model doing so has the advantage that results obtained in numerical studies can be used to understand the experimental process variables captured in the numerical simulation instance.

In this paper we study a cluster of copper particles impacting on an aluminum substrate (figure 3 [4]) and analyze further possible scenarios under which it can be used in understanding the CGDS process. The assumptions in this model were that particles are of a uniform diameter, d_p; implying a zero standard deviation on the diameter. The substrate was considered to be initially smooth compared to the size of particles used. The velocity of impact is 500m/s in the axial direction and zero in the traverse direction to the jet axis, the initial temperatures of the substrate and particles is defined to be 25 degrees Celsius, particles are assumed to be 10 um in diameter.

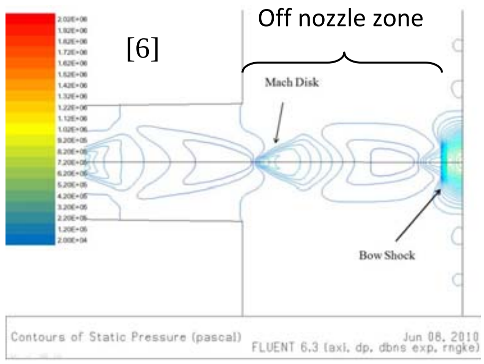
EXPERIMENT/CFD
Off nozzle process parameters

The properties of the particles Including materials for substrate and particle sizes (statistical distribution of particle size and shape); propellant gas pressures; etc.

Flight mechanics

Particle flow fields and velocity profile across off nozzle; preferred trajectories for various particle sizes

Interaction with the substrates The process parameters (Experimental) plan: the $x - y$ motion, nozzle size, feeder system, transport system, flux density, and irradiation techniques



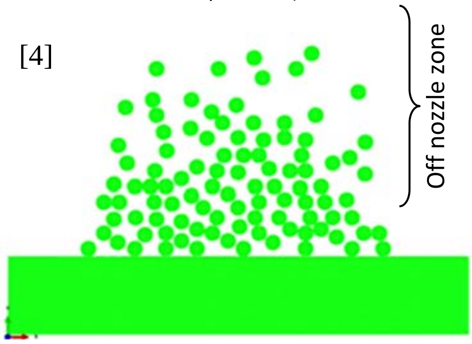
NUMERICAL PROCESS must capture the off nozzle process parameters

Input parameters in a cold spray process Including materials for substrate and particles

Defined by either: Continuum Material properties: definition of material properties through constitutive equations (Johnson cook Plasticity models; Viscoelastic, viscoplastic; Heat and Mass transfer);

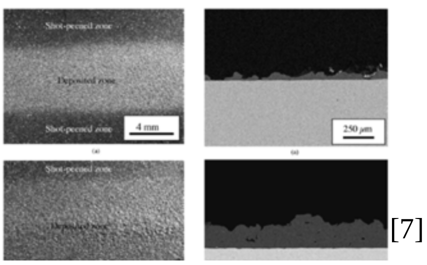
Or Molecular dynamics: for example numerical optical glass material processing, ensembles; force fields

Interaction with the substrate defines process parameters (Numerical) plan: the $x - y$ motion, nozzle size, feeder system, transport system, flux density, irradiation techniques (defines initial velocities and initial temperatures)



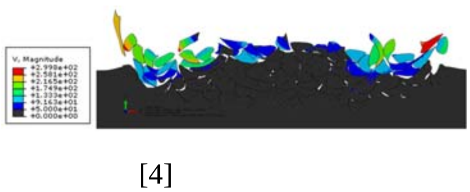
RESULTS: EXPERIMENTAL COATINGS

Output Parameters; film thickness, surface roughness, interface roughness, grain sizes, residual stresses, etc



RESULTS: PREDICTED COATINGS

Output Parameters; film thickness, surface roughness, interface roughness, residual stresses, porosity



Compare outputs to numerical result taking into consideration limitations in numerical and computational models

Figure 2. Parameter Search and System Identification Process Flow Chart.

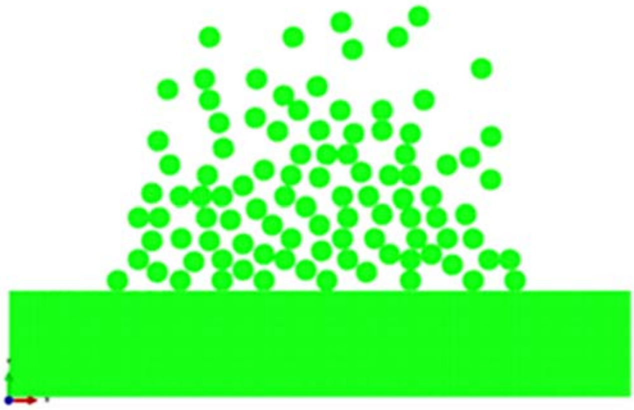


Figure 3. Computational domain, (meshing resolution of 1/20, where $d_p = 10\mu m$ particle diameter) showing a cross sectional length, part of a cross sectional length of the nozzle [4].

The simulations are based on the continuum material models using the Johnson-Cook constitutive equations [8] which define the yield flow stress, $\overline{\sigma}$ of the material as follows

$$\overline{\sigma} = \left[A + B\left(\overline{\varepsilon}^{pl}\right)^{n}\right]\left[1 + C\ln\left(\frac{\dot{\overline{\varepsilon}}^{pl}}{\dot{\varepsilon}_0}\right)\right]\left(1 - \hat{\theta}^{m}\right) \quad (1)$$

where A, B, n, C, and m are material specific constants, $\overline{\varepsilon}^{pl}$ is the effective plastic strain, $\dot{\overline{\varepsilon}}^{pl}$ is the strain rate, $\dot{\varepsilon}_0$ is the reference strain rate, $\hat{\theta}$ is the dimensionless temperature parameter defined as:

$$\hat{\theta} \equiv \begin{cases} 0 & \text{for } T < T_t \\ \frac{(T - T_t)}{(T_m - T_t)} & \text{for } T_t \leq T \leq T_m \\ 1 & \text{for } T > T_m \end{cases} \quad (2)$$

where T is the current temperature, T_m is the melting temperature of the material, and T_t is the transition temperature which defines the temperature below which the resultant yield stress is considered to be temperature independent.

3. Analysis of the findings

In this model it was observed that the mean time to impact between two consecutive particles at the same axial location was less than the time for a single particle deformation. A rotational couple and oblique trajectory are prominent characteristics in the jetting region (figure 4). These material and particle jets have higher rebound energy than those with only longitudinal velocity components. In order to have a higher deposition efficiency, η_{beam} (close to 100% deposition efficiency), selection of propellant gas pressures and nozzle characteristics should be tailored to reduce the transverse velocity component while increasing the longitudinal velocity component. For the high flux density case, this could be done by reducing the flux density or increasing the longitudinal velocity component to such an extent that the adhesion energy counteracts the jetting components.

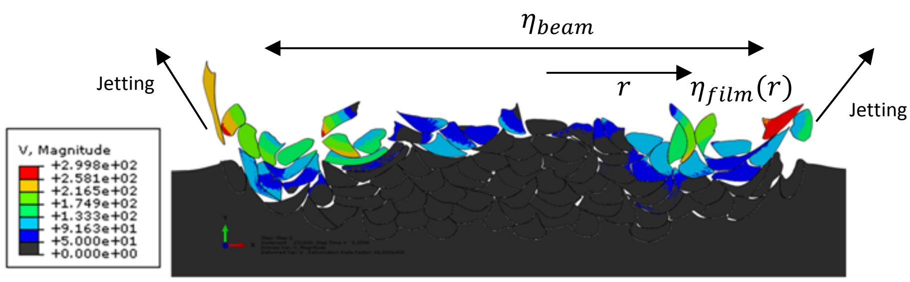


Figure 4. Rebound velocities and local deposition efficiency at a radial distance r from axis of nozzle.

Given r as a radial distance from the axis of a nozzle, and R as the maximum radial distance reached by the particles on the underlying substrate surface, the results indicate that increasing the flux density of a cluster beyond a certain limit (yet to be identified) creates a deformation behavior closely related to that of a single particle, however this process lowers the deposition efficiency $\eta_{film}(r)$ as r approaches R where R is the radius of the nozzle particle flux distribution radius at impact and r is measured from the center axis, (where $r = 0$) to towards the peripheral (where at $r = R$).

A similar characteristic on the morphology of the surfaces is observed when particles have a varying particle size: the smaller particles hit the target substrate at the peripheral at an angular velocity and possibly with reduced longitudinal velocity component and eject outward due to the oblique impact. The two scenarios (higher flux density on one hand and reduced flux density but with varying particle sizes on the other hand) are similar in terms of particles in the peripheral regions having traverse velocity components. These findings have potential applications in fabrication of functional surfaces for various applications and provide us with control variables necessary for modifying the surfaces. This analysis is also capable of prediction of agglomerate impacts of nano particles and likely morphology after impact of the agglomerate showing disintegrations of particles at the peripheral.

We therefore show that indeed the flux density and particle trajectories have a significant influence in the surface morphology. Importantly, and for future study, is to determine the settings for a 100% deposition efficiency (if at all it exists) which would yield a compact coating and also a smooth surface. It is the first time that this is being reported in the cold spray community about the influence of flux density and particle flight trajectories to surface properties of the cold spray coatings. In future, based on these findings, an analytical model for deposition efficiency can be formulated.

4. Conclusion

This paper described a simulation of the particle deposition process in a cold gas dynamic spray system and analyzing the findings show the influence of flux density to deposition efficiency and also the particle distribution and their preferred trajectories provide their contribution to reduced deposition efficiencies in cold spray systems. Deposition efficiency has been found to control the surface morphology by increased surface roughness with reduced deposition efficiency. In this analysis we took a systems approach to the problem. We also applied the concepts of data mining by collecting and analyzing observed structure in available experimental data. The numerical results were used to explain the underlying mechanics.

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