MODELLING THE FORMATION OF A THERMAL SPRAY COATING USING A STOCHASTIC APPROACH

Mohammad P. Fard [*1], Ali R. Teymourtash [*2] and Ebrahim Kamali [*3]

Department of Mechanical Engineering, Ferdowsi University of Mashhad, Mashhad, Iran
[*1] mpfard@um.ac.ir [*2] teymourtash@um.ac.ir [*3] ebkamali@gmail.com

ABSTRACT: *In this paper, a 3-D stochastic model is presented to predict the coating thickness and porosity in a thermal spray coating process. The model is based on prescribed rules in calculating the splat size during the impact of individual droplets on the substrate. Due to thermal stresses, the edge of the splats is curled up. This mechanism was assumed to be the sole reason for the porosity formation. Simulations are performed for a small section of a substrate on which a thermal spray of alumina droplets and other material particles are examined. The computed thickness and porosity were found to be in good agreement with those reported in the literature.*
Keywords: Stochastic model, Thermal spray process, Coating formation, Coating porosity, Coating thickness.

1. INTRODUCTION

Thermal spray coating is a particulate deposition process in which powders of a material are injected into a high temperature flame region where they are melted and propelled towards the surface of a substrate where individual molten particles impact, cool and solidify to form a deposit. This technology is used to produce coatings for wear, thermal, oxidation, and corrosion protection. The coating quality obtained during thermal spraying depends greatly on the dynamics of flattening of the molten particles.

Inspection of a cross section through a thermal spray coating shows that it is built up of thin lamellae formed by flattened droplets that land on each other and fuse together. Closer examination shows that the coating is not fully dense and pores are found at the interface between splats. The presence of these pores may or may not be desirable, depending on the purpose of the coating so it is important to be able to produce the desired porosity by controlling the deposition process. Extensive theoretical, experimental and numerical studies have been reported in the literature to better control this process [1]. The ultimate goal of research efforts in this field is to establish predictive correlations between the processing parameters and the properties of the coatings. Modelling the build-up of a coating formation from the impact of individual droplets can only be performed using stochastic models less reported in the literature. Cirolini et al. [2] simulated coating deposition with a two dimensional stochastic model without considering the splat curl-up and used a set of complex rules to represent interaction between the splats. Ghafouri-Azar et al. [3] used a Monte-Carlo approach to model 3D coating formation assuming a normal distribution for the spray parameters. Belashchenko and Chernyak [4] used a stochastic approach to optimize thermal spray coatings. Their modeling results are in reasonable agreement with bond strength test data for the plasma-, arc-, and flame-spray processes as well as wear resistance data for arc-sprayed steel coatings. In this study, we developed a 3D stochastic model based on a Poisson distribution for the spray parameters and a new method for the splat curl-up to predict the microstructure and thickness of thermal spray coatings.

2. MATHEMATICAL DESCRIPTION

2.1. Stochastic Model

Four main assumptions used in the stochastic model are: spray droplets are non-interacting point particles; each droplet has a different size, velocity, and impact position; the spray is random; and the probability of obtaining a droplet occurrence at any instant is independent of other droplets occurring at other instants. It is also assumed that the impact position follows a uniform distribution and the droplet specified diameter and velocity follow a Poisson distribution with a user-specified mean (λ) and standard deviation (σ) as:

$$f(s;\lambda) = \frac{e^{-\lambda}\lambda^{k}}{s!}, \quad f_{Poisson}(s;\lambda) \approx f_{normal}(s;\delta=\lambda,\sigma^{2}=\lambda) \qquad (1)$$

where s is the stochastic parameter and δ is the mean value of normal distribution. The Poisson distribution will approach a normal distribution if n>100 and $(n\times p)$<10 where n is the number of occurrences and p is the probability of occurrence. A normal distribution was used by Ghafouri-Azar et al. [3] for the velocity and the logarithm of diameter. To generate random Poisson-distributed numbers for droplet parameters, we used the FORTRAN library written by Ahrens and Dieter [5].

2.2. Splat Deposition Model

A complete coating-formation model is complex due to time scales in the order of micro seconds and spatial scales ranging from a few micrometers to a few millimeters. In the model, we need to generally deal with: molten droplets at impact with their rebound, deposition, or splashing; a single particle flattening with the consideration of solidification before the end of flattening and possible splashing; a single splat cooling with nucleation at a hyper cooling temperature; and splat layering and deposition process. The present model considers only flattening with solidification without splashing and rebounding. The diameter and velocity of droplets and their impact location are introduced randomly as mentioned above. It is assumed that droplets impinge and spread on the substrate one after another. The model assumes that a spherical droplet spreads to form a cylindrical disc of diameter d_{max} as shown in Fig. 1. Thus, the effects of any droplet splashing and breakup are neglected.

In the model, a set of rules is used to specify the final splat shape as a function of droplet impact conditions. These rules, available in the literature [6,7], are obtained using a numerical/analytical solution of droplet spreading and solidification. The solution is based on the energy conservation law: the initial kinetic and potential (surface tension) energies of a droplet before impinging on the substrate are dissipated by the viscosity and surface deformation during the impact. Final splat shapes are characterized by dimensionless numbers known as Reynolds (Re), Weber (We) and Stefan (Ste). We used following relation for spread factor $\zeta_{\max}$ [3,6,7]

$$\xi_{\max} = \frac{d_{\max}}{D} = \sqrt{\frac{We + 12}{3(1-\cos\theta) + 4(We/\sqrt{\mathrm{Re}}) + We\sqrt{\frac{3}{4}\frac{Ste}{Pe}}}} \tag{2}$$

where D is diameter, θ contact angle, Pe=Re.Pr and

$$\mathrm{Re} = \frac{\rho V D}{\mu} \quad , \quad We = \frac{\rho V^2 D}{\gamma} \quad , \quad \mathrm{Pr} = \frac{C_l \mu}{k} \quad , \quad Ste = \frac{C_l (T_m - T_{w,i})}{H_f}$$

in which C_l is the specific heat, T_m melting point temperature, $T_{w,i}$ substrate temperature, and H_f heat of fusion. It is assumed that due to thermal stresses, the edge of the splat is curled up as seen in Fig. 1. The surface of the coating and the location of pores within it, are specified using a method known as the volume fraction [3,6]. During coating build-up, the mass conservation algorithm is enforced.

2.3. Splat Curl-up Model

The curl-up phenomenon at the edge of splats is one of the main sources of coating porosity. The degree of the curl-up is affected by several factors such as: stresses generated by mismatch of thermal expansion coefficients at the coating interface; surface tension of the liquid splat; surface roughness; and remelting. The mechanism of the curl-up is extremely complicated; therefore, few attempts have been made to qualify this phenomenon. Fukanuma [8] observed that most pores exist at the periphery of splats, starting at ~0.6 times the splat radius from its centre (Fig. 1). Ghafouri-Azar et al. [3] assumed in their model of thermal spray coating formation that all splats curl up at 0.6R from its centre. Sobolev and Guilemany [9] derived a set of analytical formula to describe the pressure distribution in a flattening droplet.

Curl-up location and magnitude depend on coating materials and impact conditions. Xue et al. [10] derived a simple analytical model to predict the curl-up angle as a function of impact parameters and material properties. Their model gives the curl up angle as [10]:

$$\theta = \arctan\left(\frac{xR\alpha\Delta T}{h_s}\right) \tag{3}$$

where x is the splat curl-up start position (0.6-0.7 times the splat radius), h_s the splat thickness, α the thermal expansion coefficient, ΔT the difference between droplet and substrate temperatures, and R the splat radius ($R=d_{max}/2$).

2.4. Porosity Calculation

Several possible sources of porosity in a coating have been defined including curling up of splats, incomplete filling of interstices during deposition [8], presence of unmelted particles in spray, satellite droplets formed by splat breakup at the time of impact, entrapment of gas between splats, and the presence of oxide layer on spray particle. These sources make the porosity sensitive to particle velocity, ambient gas pressure, particle diameter, and molten material viscosity. In this paper, only the effect of splat curl-up on porosity formation was considered. The curl-up was assumed to start at a radius equal to 60% of the splat radius with an angle specified by Equation 3. The porosity is defined as the fraction of the total volume of the coating occupied by voids [3,6]:

$$porosity = \frac{V_g}{V_g + V_m} \times 100 \tag{4}$$

where V_m and V_g are the volume occupied by solid material and voids respectively.

3. RESULTS

First, to examine the results of the stochastic model, the program is run several times for the same condition but with different random parameters. The results of these simulations are shown in Fig. 2. It is seen that the calculated porosity for 25 different runs (same case) is nearly the same. The obtained average thickness is 14.9171µm with a standard deviation of 0.4164. For all simulations presented in this paper, the average values of 25 runs with different random parameters were used as the final result.

The evolution of coating formation for a thermal spray process is shown in Fig. 3 where the cross-sectional areas of the final coating are also displayed. The variation of the coating thickness in the figure is shown with color range; pores within the coating can be clearly seen as holes in the cross sections. The surface roughness is also visible in the figure. This coating was formed by impinging 500 alumina droplets with a mean diameter of 40 µm and a mean velocity of 100 m/s on a steel substrate at 800 K. The program was run for 25 times; the average results obtained are: porosity=8%, maximum thickness=110 µm and average thickness=70 µm.

For a substrate temperature of 500 K, the results of the model for droplets of various materials with a mean velocity of 100 m/s and a mean diameter of 50 µm are shown in Fig. 4. The amount of x (Eq. 3) was assumed to be constant for all cases. The difference in the porosity values for different materials can be attributed to the droplet physical properties namely the surface tension and viscosity.

Finally to validate the model, the calculated results for a thermal spray process are compared with those of the measurements [1]. As seen from Table 1, a good agreement is obtained between calculated and measured values of the porosity. The results for another set of experiment are also compared with measurements [11]. As seen from Table 2, the calculated porosity for different cases with different substrate temperatures, are within the range reported in the experiments [11].

References

[1] Pawlowski L., *The science and engineering of thermal spray coatings*, 1st ed., John Wiley&Sons, 1995.

[2] Cirolini S., Harding H., and Jacucci G., "Computer Simulation of plasma-sprayed coatings deposition model", Surf. Coat. Technology, 48, 1991, 137-145.

[3] Ghafouri-Azar R., Mostaghimi J., Chandra S. and Charmchi M., "A stochastic model to simulate the formation of a thermal spray coating". J. of Thermal Spray Technology, 12(1), 2003, 53-69.

[4] Belashchenko V.E. and Chernyak Yu. B., "Stochastic approach to the modeling and optimization of thermal spray coating formation", J. of Thermal Spray Technology. 2 (2), 1993, 159-164.

[5] Ahrens J.H., and Dieter U., "Computer Generation of Poisson Deviates From Modified Normal Distributions", ACM Trans. Math. Software, 8(2), 1982.

[6] Pasandideh-Fard M., Bhola R., Chandra S. and Mostaghimi J., "Deposition of tin droplets on a steel plate: simulation and experiments". Int. J. of Heat and Mass Transfer, 41(19), 1998, 2929-2945.

[7] Mostaghimi J. and Chandra S., "Splat formation in plasma-spray coating process". Pure Applied. Chemistry, 74 (3), 2002, 441-445.

[8] Fukanuma H., "A Porosity Formation and Flattening Model of an Impinging Molten Particle in Thermal Spray Coatings", J. Thermal Spray Technology, 3(1), 1994, 33-44.

[9] Sobolev V.V. and Guilemany J. M., "Droplet-substrate impact interaction in thermal spraying", Journal of Material Letter, 28, 1996, 331-335.

[10] Xue M., Chandra S. and Mostaghimi J., "Investigation of splat curling up in thermal spray coatings", J. of Thermal spray Technology, 15 (4), 2006, 531-536.
[11] Abedini A., Pourmousa A., Chandra S. and Mostaghimi J., "Effect of substrate temperature on the properties of coatings and splats deposited by wire arc spraying", J. Surface and Technology, 201(6), 2006, 3350-3358.

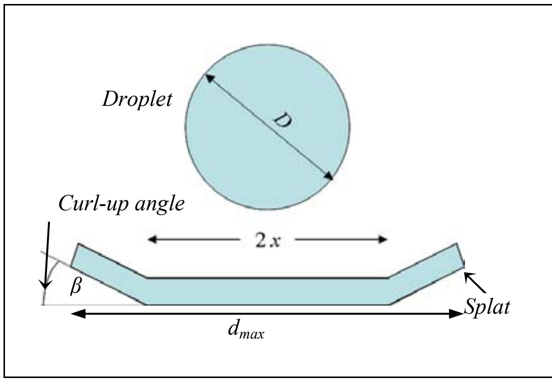

Fig. 1 A schematic of the droplet before the impact and the formed splat after the impact

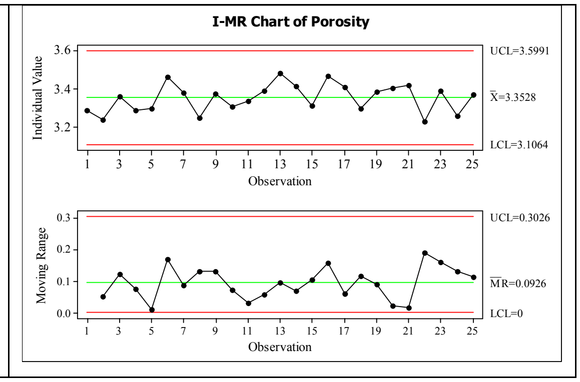

Fig. 2 The calculated porosity for 25 runs of the program for one case; the average porosity is 3.3538 with a standard deviation of 0.0734.

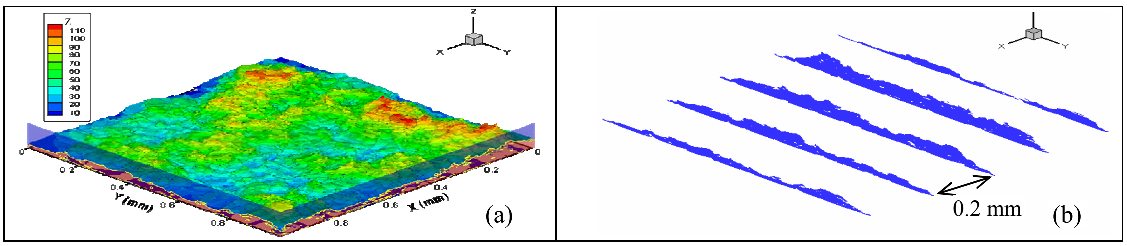

Fig. 3 Model results for a typical thermal spray process: a) the final coating topology and b) several cross-sectional areas. The porosity obtained in this case was 7%.

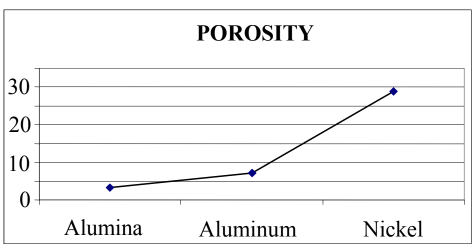

Fig. 4 The effect of spray materials on coating porosity

Table 1. A comparison between model predictions and measurements [1].

	Experiments	Model
Material	Alumina	Alumina
Mean diameter (μm)	-63+16	63
Mean velocity (m/s)	125	125
Porosity%	6.8	7.23
Ave. thickness (μm)	----	55.7
x	---	0.6

Table 2. Model results compared with measurements [11] for a thermal spray process (aluminum on stainless steel) with different conditions.

Substrate Temp. (ºC)	Porosity (%)			
	Case 1 (V_{av}=143±3 m/s)		Case 2 (V_{av}=109±2 m/s)	
	Measurements	Model Results	Measurements	Model Results
100	---	---	0.9 - 2.5	1.626
150	---	---	0.7 - 3.1	1.630
200	0.9 - 1.3	2.143	0.2 - 3.6	1.631
250	0.8 - 3.5	2.148	1.8 - 3.8	1.634
300	2.2 - 2.4	2.139	2.5 - 4.1	1.628