A STOCHASTIC MODEL OF PLASMA SPRAYED COATING FORMATION

R. GHAFOURI-AZAR, J. MOSTAGHIMI, AND S. CHANDRA
CENTRE FOR ADVANCED COATING TECHNOLOGIES
DEPARTMENT OF MECHANICAL AND INDUSTRIAL ENGINEERING
UNIVERSITY OF TORONTO
TORONTO, ONTARIO, M5S 3G8 CANADA

Abstract

Physical properties of plasma sprayed coatings, e.g., porosity, surface roughness and thickness, are sensitive to a large number of process parameters such as droplet size distribution, velocity, temperature and impact point. Finding spray operating conditions that yield the best coating structure requires considerable trial and error. To reduce this effort we need a fundamental understanding of spray coating formation. In this study we have developed a stochastic, three-dimensional (3-D) model of coating formation. The properties of impacting particles are assumed to vary stochastically using a normal probability density function. Splat peripheral detachment is assumed to be the source of porosity formation. The model is able to predict coating porosity, thickness and roughness as a function of spray parameters.

Introduction

Plasma sprayed coatings consist of lamellar splats interspersed with pores. Splats - which are formed by the impact, spreading and solidification of individual droplets onto the substrate - are the fundamental building block of the coating. Depending on the shapes of splats and the nature of their interactions, different types of microstructure, varying porosities, and consequently different coating properties are obtained.

Splat shape depends on many factors such as size, velocity and thermophysical properties of the impacting particles, as well as the topology and properties of the substrate. On-line measurement of these parameters for all impacting particles would be enormously complex, but their statistical distributions can be easily determined.

Several studies have investigated the nature of thermal spray coating and formation of splats [1-3]. To date, the vast majority of these studies have been concerned with predicting the behaviour of a single particle impacting onto a flat surface [4-10]. Cai and Lavermia developed an analytical model of coating formation in which either shrinkage of splats during solidification, or interstitial porosity, were considered to be possible sources of porosity [11]. Other studies [12-14] employed the Monte Carlo approach, assuming a two-dimensional (2-D) domain that represented a cross-section through the thickness of the coating. Porosity was assumed to be created as a result of gaps between splats or splat curl up. Kanouf et. al. [15] developed a model which considered the effect of spraying angle on coating roughness. The model estimated an unrealistically large roughness and it could not predict porosity. To date, all published models of coating formation have been 2-D, though in reality coating deposition is a complex, 3-D process.
In this paper we describe the development of, and results from, a 3-D stochastic model of plasma spray coating formation. We assume that the mean values and standard deviations of droplet size $D$, velocity $V$, temperature $T$, impact point $(r, \Theta)$ and degree of splat edge curl up $\alpha$ are known. Based on probability density functions - assumed to be normal - we estimate the instantaneous process parameters for each impacting particle and calculate splat sizes. At present the splat size is predicted analytically. Droplets are assumed to spread after impact and form disks whose edges curl up due to thermal stresses. This is assumed to be the primary source of porosity. The model is used to predict coating porosity, thickness and roughness as a function of spray parameters.

Methodology

**Stochastic analysis**

We assumed process parameters have normal distributions, given by:

$$g(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{1}{2\sigma^2} (x - \beta)^2 \right) \quad (7)$$

For each distribution, the mean value $\beta$ and the standard deviation $\sigma$ are specified using experimental data. We assign mean values to the process parameters, $\bar{X} = [\bar{V}, \bar{r}, \bar{\Theta}, \bar{D}, \bar{\alpha}, \bar{F}]$ and a standard deviation $\sigma_{\bar{X}} = [\sigma_{\bar{V}}, \sigma_{\bar{r}}, \sigma_{\bar{\Theta}}, \sigma_{\bar{D}}, \sigma_{\bar{\alpha}}, \sigma_{\bar{F}}]$ corresponding to each of these variables. We assume these parameters are independent of each other.

To derive an explicit relation between the normal random variable and probability density function we use a cumulative distribution function $F(x)$, calculated by integrating the probability density function within the desired limits, i.e.,

$$F(x) = P(a < x \leq b) = \frac{1}{\sigma \sqrt{2\pi}} \int_a^b \exp \left( -\frac{(x - \beta)^2}{2\sigma^2} \right) dx,$$

or by changing the variable to the random variate $t = (x - \beta) / \sigma$, we have

$$F(t) = P(t_1 < t \leq t_2) = \frac{1}{\sqrt{2\pi}} \int_{t_1}^{t_2} \exp\left(-\frac{t^2}{2}\right) dt,$$  

Carrying out a numerical integration, we correlated the variation of $F(t)$ versus $t$. To assign an input variable, we generated a uniformly distributed random number between $(0,1)$. Then, the random variate $t$ was estimated by substituting the cumulative distribution function for the random variable. With the mean value, standard deviation and random variate, the coating parameter was evaluated stochastically: e.g., $X = \bar{X} + t\sigma_{\bar{F}}$.

**Splat shape**

When a particle lands on a flat surface, different splat shapes are possible. The droplet may become a circular disk splat, segments of whose periphery detach; it may form an irregular splat with fingers projecting around its rim; or it may splash, shattering into small
satellite particles. Figure 9 shows photographs of splats formed during plasma spraying of nickel powders onto a stainless steel surface, illustrating these different outcomes.

Splat shape is controlled by inertial, viscous and surface tension forces in the spreading molten droplet, substrate geometry, liquid-solid contact angle, heat transfer between the droplet and substrate, and substrate thermal properties. Droplet spreading and solidification are governed by the interplay of these parameters.

![Figure 9 Nickel splat shape at different impact condition.](image)

As a first step in the development of our model, we neglected the effects of droplet splashing and break-up. We estimated the diameter of a splat formed by the impact and solidification of a molten droplet from an analytical model [5]. The maximum spread factor $\xi_{\text{max}}$, defined as the ratio of the splat diameter $d$ to that of the droplet $D$, is a function of the Weber number $We = \rho v^2 D / \gamma$, Reynolds number $Re = \rho v D / \mu$, Stefan number $St = C(T - T_s) / H_f$, and Peclet number $Pe = vD / \alpha$:

$$\xi_{\text{max}} = \frac{We + 12}{\sqrt{4 We + We \sqrt{\frac{3 St}{4 Pe}}} \quad (10)}$$

The thickness of the splat $h$ is given by $h = \frac{2D^4}{3d^3}$.

The splat shapes of droplets landing on an uneven surface are highly sensitive to the surface topology. Comparison of splat shapes formed when a molten tin droplet is dropped on a previously deposited splat shows that the relative position of the two droplets has significant effect on the final shape of splat. Figure 10 shows the sequential deposition of two droplets where the shape of the second striking droplet changes dramatically with different spacing between droplet centers.

![Figure 10 Photographs of the offset deposition of two tin droplets.](image)

**Coating formation**

We used a 3-D mesh to define the computational domain and to tracking the shape and position of the coating surface. A deposited splat was completely described by its position
coordinates \((r, \Theta)\), diameter and thickness. We assumed that curling-up of the splat periphery was the source of porosity; curling was confined to the portion of the splat lying between \(0.6R\) and \(R\) [16] with its magnitude described by the angle \(\alpha\) illustrated in Figure 11.

The coating structure was described in the model by the "volume fraction" \((f_i)\), defined as the fraction of the volume of each cell \((V_{cell})\) occupied by coating material (with volume \(V_m\)). In discretized form, the volume fraction of a cell with coordinates \(i, j, k\) is

\[
f_{i,j,k} = \frac{V_m}{V_{cell}} = \frac{\int_{x_{i,j,k}} f_{x,y} \, dx \, dy \, dz}{\Delta x \cdot \Delta y \cdot \Delta z} \tag{11}
\]

where

\[
f_x = \begin{cases} 
1 & \text{inside the splat} \\
0 & \text{outside of splat}
\end{cases} \tag{12}
\]

Hence, \(f_{i,j,k}\) equals unity when the cell is filled with material, zero when the cell is empty and \(0 < f_{i,j,k} < 1\) when the cell contains voids or a free surface.

![Figure 11 Schematic diagram splat deposition and coating formation](image)

Droplet interactions were modelled by assuming four different splat shapes could be produced by the impact of a droplet on an already deposited splat. These were based on pictures taken during experiments on the sequential impact of tin droplets (Figure 11) where the final splat shape was found to depend on the offset between droplet centres. After a particle was deposited, the shortest distance between its impact point and the centre of the nearest previously deposited splat was determined. This distance was used to define the shape of the final splat.

Coating growth is a result of splat agglomeration. It was assumed that each splat at the time of deposition completely filled all cavities under the flat portion of the splat. As depicted in Figure 11, all material lying between \(0 \leq X_{i,j} < 0.6R\) for each splat was completely transferred to the last cell below it, without any pores. If \(0.6 \leq X_{i,j} \leq R\), (corresponding to the curled up edges of the splat), the material of the cells, plus any included voids, were moved to the top of the last filled cell directly below. Summing up \(f\) values from all deposited splats described the coating and the pores within it.

**Movement of spray gun**

In a real spray coating process either the spray gun, or the substrate, or both, move in order to coat the surface uniformly. Gun motion has a significant effect on the coating
topology and roughness. To reproduce this effect, we allowed the plasma gun to move in simulations. The position \( \hat{x} \) where droplets landed was calculated as

\[
\hat{x} = \hat{x}_g + \hat{x}_c, \quad (13)
\]

where \( \hat{x}_g \) denotes the gun location and \( \hat{x}_c \) the center of the splat relative to the gun. The spray gun can be programmed to have different motions, such as constant velocity, sinusoidally varying velocity, or any other arbitrary movement.

Since the time required for a droplet to spread and solidify is much less than the flight time of particles, we assume that their impact on the substrate is sequential. The time taken for each droplet to spread to its maximum extent is approximately \( t_s = 8D / (3V) \) [5]. This value was assumed to be the time between two particles landing.

**Results**

The stochastic model was applied to the deposition of nickel particles. Figure 12(a) shows the coating formed in a 300 \( \times \) 300 \( \mu \text{m} \) substrate area by a gun held stationary over the centre of the substrate. The particle parameters assumed in the simulation are shown in Table 1. The effects of gun movement on the surface profile of coating are depicted in Figure 12(b). Here gun travelled over the substrate with a constant velocity. All other parameters were the same as those in Table 1. As expected, the coating thickness was uniform for the moving gun.

![Figure 12 The effect of gun movement](image)

Cross sections through the coating gave values of the thickness, porosity and surface roughness distributions, illustrates a typical cross-sectional view of the coating microstructure. The mean thickness (\( Z_m \)) and average surface roughness (\( R_s \)) of this section are about 140 and 17 \( \mu \text{m} \) respectively. \( R_s \) is estimated from

\[
R_s = \frac{1}{L} \int_0^L |Z - Z_m| \, dx, \quad (14)
\]

![Figure 13. Typical average surface roughness \( R_s \) and average thickness \( Z_m \)](image)

![Figure 14. Variation of porosity and average thickness with particle speed](image)
<table>
<thead>
<tr>
<th></th>
<th>Velocity</th>
<th>r-Comp.</th>
<th>θ-Comp.</th>
<th>Diameter</th>
<th>Temp.</th>
<th>Curl up</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[m/s]</td>
<td>[m]</td>
<td>[Rad]</td>
<td>[μm]</td>
<td>[K]</td>
<td>[Rad]</td>
</tr>
<tr>
<td>Mean Value $\bar{X}$</td>
<td>400</td>
<td>0</td>
<td>0</td>
<td>30</td>
<td>1572</td>
<td>$\phi$ d</td>
</tr>
<tr>
<td>Stand. Dev. $\sigma_y$</td>
<td>20</td>
<td>25</td>
<td>0</td>
<td>5</td>
<td>100</td>
<td>$\phi/(2d)$</td>
</tr>
</tbody>
</table>

Table 2. Stochastic input data

where $l$ and $Z$ are the estimated roughness and surface profile thickness, respectively.

We calculated average values of the coating porosity and thickness for varying spray parameters. Figure 14 shows the variation of porosity and coating thickness with average particle speed. The model predicted a decrease in both these parameters with increasing impact speed, a trend that agrees with experimental evidence. The model also predicted that increasing average particle speed reduced surface roughness $R_y$, due to the splats being thinner at higher impact speeds.

References