Abstract
Complete modeling of plasma spray coatings involves modeling of the plasma fields, calculating particle trajectories and temperature history, and modeling the impact of molten droplets on the substrate and formation of individual splats. This paper reports on recent advances in droplet impact in plasma spray coating process.

Introduction
Plasma spray coating is a process by which the high temperature of plasma is employed to melt powders of metallic or non-metallic materials and spray them onto a substrate, forming a dense deposit (Fig. 1). The process is commonly used to apply protective coatings on components to shield them from wear, corrosion, and high temperatures. The most widely used plasma spray sources include direct current plasma (dc) and, to a lesser degree, radio frequency inductively coupled plasma (rf-ICP). The process may be at atmospheric pressure or under vacuum.

Thermal spray coatings are built up by agglomeration of splats formed by the impact, spread, and solidification of individual particles. The state of particles at the point of impact is dependent on their trajectory and residence time within the plasma. Thus, the particles may be fully or partially melted and few particles may be in solid form. Coating properties such as porosity, adhesion strength, and surface roughness depend on the shape of these splats and how they bond together and to the substrate. The splat shape is dependent on material properties of the powder; impact conditions, e.g., impact velocity and temperature; and substrate conditions, e.g., substrate topology and temperature.

Understanding the dependence of the microstructure of spray coatings on the operating conditions of the plasma spray system is of great practical interest. To obtain good quality coatings the spray parameters must be selected carefully, and due to the large variety in process parameters, much trial and error goes into optimizing the process for each specific coating and substrate combinations. A great deal of research is currently devoted to exactly understand how varying spray parameters changes coating properties. Experimentally validated mathematical models of the process play a significant role
in reducing the extent of such trial and error procedures.

**Coating Formation**

Given the impact conditions of powders on a substrate and plasma spray gun speed, Ghafouri-Azar et al. [1] and M. Xue [2] developed a stochastic model to predict coating microstructure. Sources of porosity include splat curl-up and partially filled interstices. Once an impact event is randomly selected from the given distributions of size, velocity, and temperature of the powder, the splat shape is found from an analytical formula derived by Pasandideh-Fard et al. [3]. Figure 2 shows the predicted coating structure for the atmospheric plasma spraying of yttria-stabilized zirconia (YSZ).

![Figure 2. Predicted microstructure of a YSZ coating by stochastic model [2]; porosity 11.7%, average coating roughness 5.7 μm.](image)

The model predicts porosity, thickness, and roughness of the coating. Additionally, residual stresses are also predicted [1]. The accuracy of this model depends on the accuracy of the given shape of splats, which for the above model was based on an analytical approach and the splats were all assumed to be disk-like. In the following, an accurate, computational model of Impact and solidification is described.

**Droplet Impact and Solidification**

First, let us consider the impact of a molten drop on a smooth surface. We assume that the flow is laminar and incompressible, and solidification occurs at equilibrium temperature. Furthermore, thermal contact resistance is assumed to be known. In order to predict the impact dynamics and the solidification history, a time-dependent, 3-dimensional numerical model has to be developed. The model solves the conservation equations for mass, momentum and energy. Additionally, surface tracking models are needed to resolve the deformation of the interface during the impact. Bussmann et al [3, 4] developed such a method and studied the splashing behavior in the isothermal impact of a molten tin droplet on a stainless steel surface. They showed the important effect of large (non-wetting) contact angles on splashing behavior. Mostaghimi and co-workers [5-7] extended their model and included the effect of heat transfer on droplet impact. The model included phase change and heat transfer within the substrate. The effect of density increase, which is a result of solidification, on the splat shape was modeled in [7].

One issue specific to this type of problem is tracking the liquid-gas interface. A robust technique for interface tracking is the volume-of-fluid (VOF) technique [8] with an improved Young’s algorithm [3, 9]. In the VOF method, a scalar function, \( f \), is defined as:

\[
f = \begin{cases} 
1 & \text{within the liquid phase} \\
0 & \text{elsewhere}
\end{cases}
\]

Since \( f \) is passively advected with the flow, it satisfies the advection equation:

\[
\frac{\partial f}{\partial t} + (\vec{V} \cdot \nabla) f = 0
\]

Where \( t \) is time and \( \vec{V} \) is the velocity vector. The interface unit normal is related to \( f \) by \( \hat{n} = \nabla f / |\nabla f| \) and the interface curvature is given as, \( \kappa = -\nabla \cdot \hat{n} \). There is a
pressure jump across the interface which, under equilibrium conditions, is given as
\[ \Delta p = -\sigma K \]
where \( \sigma \) is the surface tension coefficient. The pressure jump across the interface was modeled by the continuum surface force (CSF) model of Brackbill et al [10].

The model reported in references [3-7] has shown excellent agreement with experimental measurements of the impact of a tin droplet on a stainless steel substrate (Figure 2).

The predicted final shape of a molten nickel droplet at 2600 °C of 60 μm diameter at an impact speed of 73 m/s on a stainless steel substrate is shown in Fig. 3(a). The substrate was initially at 290 °C temperature. Thermal contact resistance was assumed to be constant during the impact and, based on experimental evidence, was chosen 10^{-7} m^2 K/W. In agreement with experimental observations [11], the results show that under these conditions, substantial number of fingers is formed and the droplet splashes. A careful examination of the results show that fingering and break-up is indeed induced by instabilities originating from solidification; the break-up is not due to Rayleigh-Taylor instability. When thermal contact resistance is increased by one order of magnitude to 10^{-6} m^2 K/W, heat transfer is reduced, and no splashing occurs (Fig. 3(b) and ref. [11]). Thermal contact resistance is therefore an important factor in determining the shape of splats. In general, thermal contact resistance depends on the substrate roughness, its temperature, the ambient pressure. Furthermore, although this is assumed to be constant in these calculations, in principal, it is a function of time and position. A good examination of our current understanding of the effect of the thermal contact resistant can be found in [12]. Considerable more research is needed on this subject so that an accurate predictive model for thermal contact resistance is established.

To understand the effect of roughness, Raessi et al [13] and Parizi et al [14] considered the impact of molten alumina and zirconia drops on etched surfaces, respectively, where the topology of the surface is well defined and regular. Thermal contact resistance was assumed to be zero. It was found that for a 1-μm roughness, compared to the impact on a smooth surface, the spread factor increases. This indicates that the apparent thermal contact resistance has increased and is no longer zero [14]. Again, the results show that solidification plays an important effect in determining the final shape of the splat, particularly for larger roughness, e.g., >2 µm [Fig.4].

Mehdi-Nejad et al. [15-17] considered the effect of the gas phase on the dynamics of impact. They show that under certain conditions, due to the high stagnation pressure, a gas bubble may be trapped under the impacting drop. Depending on the liquid properties, the bubble may detach and travel to the surface or it may stay on the substrate.

Chae et al [18] considered the effect of rapid solidification on the impact of alumina droplets. They showed that as a result of under-cooling effects, the spread can be considerably reduced. Study of under-cooling effect on droplet impact is the subject of current research.

**Conclusions**

Over the last 15 years, much research has been carried out to understand the dynamics of droplet impact and the effect of solidification on impact of molten drops on a substrate. Powerful numerical models have been developed and validated with carefully designed experiments. The results show the importance of solidification on splashing behavior. Thermal contact
resistance is shown to be a major factor in controlling heat transfer and solidification. Current research on the subject includes improving the surface tracking algorithms [e.g., 19], more in-depth studies of the rapid solidifications effect, effect of temperature dependent properties, e.g. density [7] or surface tension coefficient, which promotes Marangoni convection.

Finally, the available data on thermodynamic and transport properties of high melting point materials is rather limited, particularly for alloys and, as well, temperature dependence of these properties. These data are input to the models described in this work and, thus, the results depend on them. New methods for rapid measurement of such properties have to be developed [e.g., 20]. Contact angle measurements should also be pursued. Contact angles, however, depend on both droplet and substrate materials.

References
5. M. Bussmann, S. Chandra, J. Mostaghimi, Physics of Fluids, 12, pp. 3121-3132, 2000M.

Fig. 2. Evolution of the spread factor (=splat diameter to droplet diameter) for the normal impact of a 2.7 mm tin droplet initially at 240 °C impacting at speed of 1 m/s on a stainless steel plate initially at 25 °C [4]

Fig. 3. Nickel splat shapes on a steel plate: initially 290°C, contact resistance 10^-7 m²K/W (top); initially at 400 °C, contact resistance 10^-5 m²K/W [11] (bottom)

Fig. 4. Impact of Alumina on patterned surface, (a) comparison between impact on smooth, 1, 2, and 3-µm “roughness”; (b) solidification effect for 3-µm case [13].