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Numerical Simulation of Droplet Impact on Patterned Surfaces

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Abstract

In this work we present the numerical simulation results for the molten nickel and zirconia (YZS) droplets impact on different micro-scale patterned surfaces of silicon. The numerical simulation clearly showed the effect of surface roughness and the solidification on the shape of the final splat, as well as the pore creation beneath the material.

The simulations were performed using a computational fluid dynamic software, Simulent Drop, The code uses a three-dimensional finite difference algorithm solving full Navier Stokes Equation with heat transfer and phase change. Volume of fluid (VOF) tracking algorithm is used to track the droplet free surface. Thermal contact resistance at the droplet–substrate interface is also included in the model. Specific attention is paid to the simulation of droplet impact under plasma spraying conditions. The droplet sizes ranged from 15 to 60 microns with the initial velocities of 70-250 m/s. The substrate surface was patterned by a regular array of cubes spaced at 1 μm and 5 μm from each other. The peak to valley height of each cube was between 1 to 3 μm. Different splat morphologies will be compared with those obtained from the experimental results under the same impact and surface conditions.

Introduction

Liquid droplet spreading on surfaces occurs in many industrial processes such as painting, coating, ink jet printing, lubrication, and thermal spray coatings. In thermal spray coating, in order to enhance the adhesion of the impact droplets on the surface, the substrate is usually grit blasted. Therefore, the complex physical phenomena of droplet spreading and solidification take place at a microscopically rough and non-flat surface on a substrate. The surface roughness of the substrate will affect the dynamic of the droplet spread as well as the shape and the thickness of the final splat. More over, it can be shown that the initial roughness of the surface would cause splashing of the molten droplet which in turn causes more roughness on the surface layer of the additional coating. Therefore the initial roughness parameters of the surface may affect the porosity level of the coating layer.

As Raessi et al [1] explained in their work, though many experimental and numerical studies have been presented on droplet impact and solidification processes, only a few number of them considered the effect of surface roughness. Using a two dimensional axi-symmetric model Ahmed and Rangel [2] numerically studied the impact and solidification of an aluminum droplet on a wavy substrates. The average size of the droplets under their study was 600 mm with a velocity of 100 m/s. Their results show that droplet impact onto an uneven substrate is almost always accompanied by splashing which would decrease by increase in the surface roughness height. Fukanuma [3] presented a formula which describes the flattening process of a droplet onto a rough surface, and concluded that the flattening ratio and the flattening time decreases with increasing roughness. Liu et al. [4] numerically studied the impact of a droplet onto substrates with wavy surfaces; however, their two-dimensional axi-symmetric model did not include solidification. They found that for wavelengths of the surface larger than the droplet diameter, droplet spreading ended with breakup. Raessi et al [1] used a three dimensional model [5,6] to numerically simulate the effect of surface roughness on the impact dynamics and the splat shape of an alumina droplet impinging onto a substrate. They concluded that droplet solidification is the main mechanism responsible for changing the splat shape.

In this study we present the numerical modeling of deformation and interaction of molten nickel and zirconia (YSZ) droplets impinging on a textured (patterned) surface during thermal spraying. This research represents a significant advance with respect to other numerical modeling that were limited to a two dimensional studies or no solidification. One of the basic objectives on this study is to understand the

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fundamental mechanisms governing the pore formation in thermal spray coatings as well as to determine the important processing parameters on the splat shape and morphology for a metal droplet (nickel) and an oxide material (zirconia).

Numerical Model

Fluid Flow

Bussmann et al. [5] have presented a detailed discussion of the fluid flow algorithm that is used in the three dimensional code, Simulent Drop. Fluid flow for droplet impact was modeled using a finite-difference solution of the Navier– Stokes equations in a three-dimensional Cartesian coordinate system. The liquid is assumed to be incompressible and any effect of the ambient air on droplet impact dynamics is neglected. The fluid flow is assumed to be laminar. The free surface of the deforming droplet is tracked using the volume of fluid (VOF) scheme described in [5]. In this method, a scalar function f is defined as the fraction of a cell volume occupied by fluid. f is assumed to be unity when a cell is fully occupied by the fluid and zero for an empty cell. Cells with values of $0 < f < 1$ contain a free surface. Surface tension was modeled as volumetric force acting on fluid near the free surface; the method used was the continuum surface force (CSF) model integrated with smoothed values of function f in evaluating free surface curvature. Tangential stresses at the free surface were neglected. Contact angles were applied as a boundary condition at the contact line.

Heat Transfer

The heat transfer in the droplet and in the substrate was modeled by solving the energy equation, neglecting viscous dissipation. Passandideh-Fard et al [6] presented more details about this model. Heat transfer in the droplet and substrate regions were coupled through the heat flux q at the droplet–substrate interface. For the portions of the substrate not covered by the droplet it is assumed that there was no heat transfer so that $q = 0$. Where the droplet and substrate are in contact, however,

$$q = \frac{(T - T_W)_{Substrate}}{R_C} \qquad (1)$$

where R_C is the thermal contact resistance between droplet and substrate per unit area. Values of R_C are provided as an input to the model. Although in principle R_C could vary with both time and position, we used a constant value in the simulations.

Liquid density and surface tension were assumed constant. Liquid viscosity and substrate thermal properties, however, were assumed to vary with temperature. Properties of nickel and silicon are well documented such as in [7]. Properties for molten YSZ droplet are less investigated. The methods and values presented by Shinoda et al [8] and Simon and Pal [9] have been used in this work.

Governing Equations

Equations of conservation of mass and momentum for the flow are:

$$\nabla . \mathbf{V} = 0 \qquad (2)$$

$$\frac{\partial \mathbf{V}}{\partial t} + \nabla .(\mathbf{V}\,\mathbf{V}) = -\frac{1}{\rho}\nabla p + \nabla^2 \nu\, \mathbf{V} + \frac{1}{\rho}\mathbf{F}_b \qquad (3)$$

where $\mathbf{V}$ represents the velocity vector, p the pressure, ρ the density, ν the kinematic viscosity, and $\mathbf{F}_b$ any body forces acting on the fluid, including the surface forces.

By neglecting viscous dissipation and assuming that the densities of liquid and solid are constant and equal to each other, the energy equation can be represented by:

$$\frac{\partial h}{\partial t} + (\mathbf{V} \cdot \nabla) h = \frac{1}{\rho} \nabla \cdot (k \nabla T) \qquad (4)$$

where h is the enthalpy of the fluid, k the thermal conductivity, and T is the temperature.

Since the scalar function f is passively advected with the flow, f should satisfy the advection equation as well:

$$\frac{\partial f}{\partial t} + (\mathbf{V} . \nabla) f = 0. \qquad (5)$$

Given the volumetric nature of f and in order to maintain a sharp interface, the discretization of the above equation requires special treatment. Youngs' algorithm is used to track the free surface. It consists of two steps: an approximate reconstruction of the interface followed by a geometrical evaluation of volume fluxes across cell faces. More details can be found in [5,6].

In Fig. 1, the schematic set up for the numerical simulation of a droplet impact on a uniform textured surface is shown. Thought the roughness created on the surface by grit blasting is a random roughness, numerical modeling with a well defined roughness model can provide valuable information about the spreading and solidification behavior of the droplet.

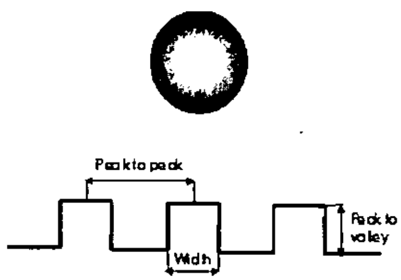


Figure 1: The schematic set up for simulation of the droplet impact on a patterned surface. The major parameters define the surface roughness are: Peak to peak distance, width, and peak to valley distance (height) of the cubes. Throughout this paper, "space" between cubes indicates the peak to valley minus the width of each cube.

Experimental Parameters

In order to directly compare the simulation results with the experimental observation, the impact parameters were chosen as those used or measured in the experimental set ups.

The impact experiments for nickel droplets on textured silicon were performed at Industrial Materials Institute Lab in National Research Council of Canada. More details are stated elsewhere [10]. The experimental parameters for nickel are presented in Table 1.

The substrates were silicon wafers that were patterned with micron-sized columns to make a textured rough surface. The column heights were 1 µm and the spaces between the columns were either 1 µm or 5 µm. The wafers were heated to 350°C during spraying. The contact resistance between the substrate and the splat was calculated by measuring the average cooling rate between splats and textured silicon wafers.

Table 1: In flight parameters for nickel particles as measured during experiments.

Nickel on Silicon	1 µm height 1 µm space 4 µm width	1 µm height 5 µm space 4 µm width
Initial Diameter, µm	50 ± 3	60 ± 3
Initial temperature, °C	2390 ± 70	2225 ±20
Initial velocity, m/s	70 ± 2	73 ± 2
Substrate temperature, °C	350	350
Contact resistance, m^2-K/W	5.E-6 *	2.E-6 *

*Average measured values.

Table 2: In flight parameters for Zirconia particles as measured during experiments.

Zirconia on textured silicon	3.3 µm height 5 µm space 4 µm width	1.5 µm height 5 µm space 4 µm width	
		(a)	(b)
Initial Diameter, µm	15	15	15
Initial temperature, °C	2900	2700	2900
Initial velocity, m/s	250	250	250
Substrate temperature, °C	25	25	30
Contact resistance, m^2-K/W	1.E-8	1.E-7	1.E-8

The experiments with zirconia were performed at the Center for Advanced Coating Technologies at the University of Toronto. In-flight particle conditions upon impact were measured with a DPV-2000 monitoring system (Tecnar Automation Ltee, St-Bruno, Canada). It simultaneously calculates the diameter, velocity and temperature of the particle. The in flight parameters for zirconia are shown in Table 3. The values of thermal contact resistance are obtained numerically by comparing the simulation results and the experimental observation.

The substrates were silicon wafers with micron-sized columns of heights 3.3 µm and 1.5 µm. The spaces between the columns were 5 µm and the width of columns equal to 4 µm. The wafers were kept at room temperature during spraying.

Results and discussions

Nickel Droplet Impact

Figures 2, and 3, show the normal view and close up of the nickel splat on the silicon patterned surface. The top picture shows the simulation results and the bottom picture shows the SEM image of the splat from the experiment.

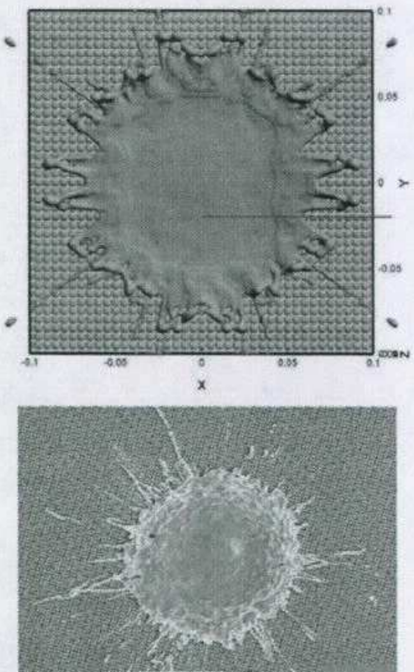


Figure 2: The numerical result (top) for a splat shape of nickel on silicon with 1 µm high and 1 µm spacing between the cubes. Other impact parameters are stated in table 1. Bellow is an SEM image of the splat taken from experiments almost at the same conditions.

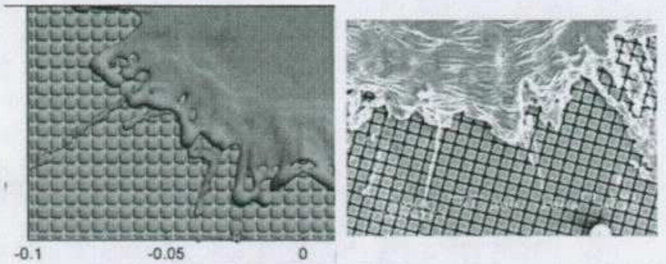


Figure 3: Close up of the splat shape at the rim of splat for Fig. 2.

The final splat diameter obtained from the simulation was 180 μm which is comparable with the value of 195 μm measured from the experiment. Figure 4, shows the normal view of nickel splat on 1μm height, 5 μm textured silicon and corresponding SEM image. In Fig. 5, a close up image of the splat boundary and corresponding SEM image is shown as well. The maximum diameter in this case was obtained from measurement as 175 mm which is in good agreement with the calculated value of 170 microns.

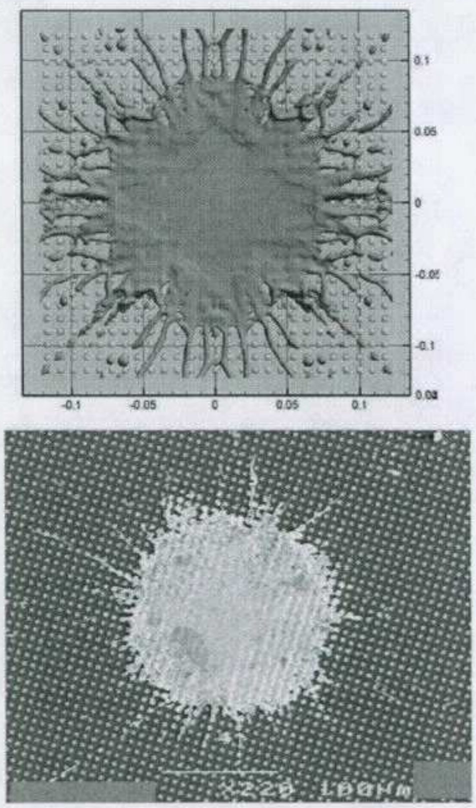


Figure 4: The numerical result (top) for a splat shape of nickel on silicon with 1 μm high and 5 μm spacing between the cubes. Other impact parameters are stated in Table 1. Bellow is an SEM image of the splat taken from experimental conditions almost at the same conditions.

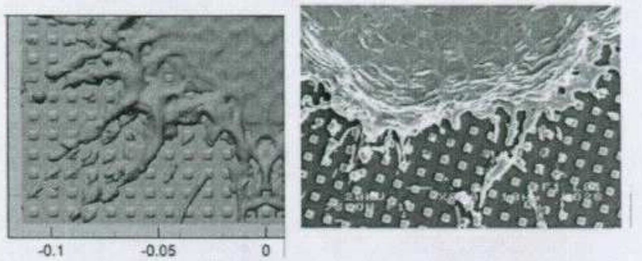


Figure5: Close up of the splat shape at the rim of splat for Fig. 4.

Figure 6, top, shows the cross section of the splats and the substrate, at the location shown with a red line in Fig. 1. As it is seen from the figure, the cavities between the textured posts on the substrate are filled with the droplet material in the middle of the splat, whereas close to the boundaries of the splat the cavities are partially filled or completely open. In the bottom part of Fig.6, the focused ion beam (FIB) image of one nickel splat, sprayed almost under the same condition is shown. As can be seen from the close up image, most of the posts in the middle of the splat are also filled with nickel. This is a clear indication that closed to the impact point of the droplet, where the kinetic energy of the liquid and its normal velocity are at highest the cavities on the surface are filled up regardless of the size. As the normal velocity of the liquid reduces and liquid spreads in radial direction, the liquid energy is not enough to fill the cavities.

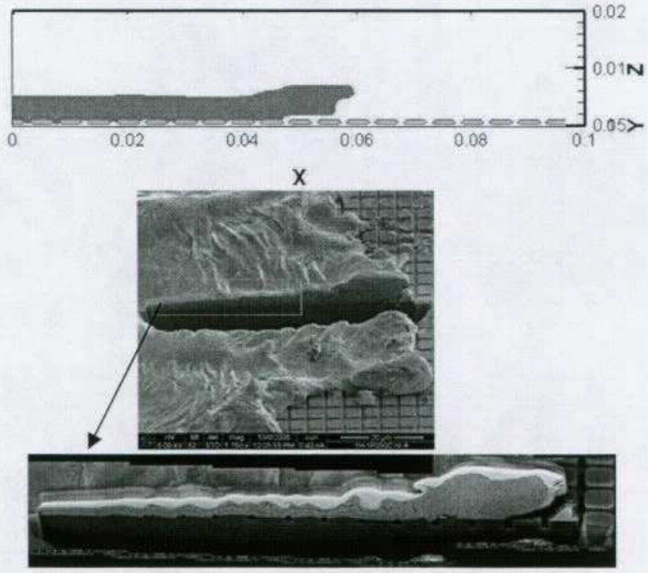


Figure 6: Top: Cross sections of nickel splat, corresponding to Fig. 2 at the location indicated by red line. Bottom: FIB image from the nickel splat under the same conditions. The close-up of the cut shows that the posts close to the center of the splat are filled with material. The same feature can be seen from the simulation results.

Zirconia Droplet Impact

Figure 7, shows the simulation results of a 15 μm molten zirconia droplet impact on the textured silicon surface of 3.3 μm height and 5 μm space between cubes. Other impact conditions are stated in Table 2. This figure also shows the cross section of the splat at the location with the red line on the top picture. The initial velocity of the droplet in this case was more than three times of the nickel splat (250 m/s). Also the roughness parameters, i.e., peak to peak, and peak to valley distances are comparable with the droplet size. As can be seen the shape of the splat in this case is closer to square shape than a round shape and most of cavities in between the roughness posts are filled with the material

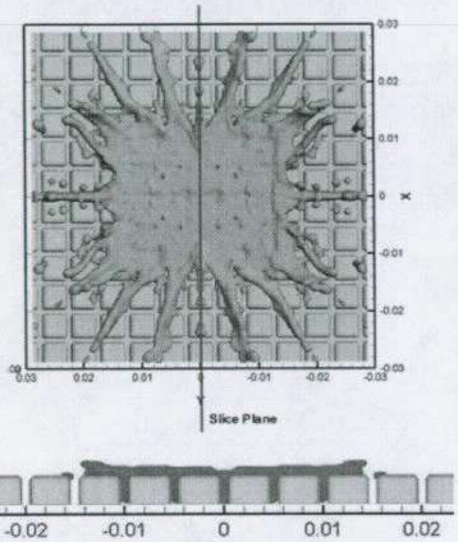


Figure 7: The numerical result of a splat of YSZ on silicon. Other impact parameters are stated in table 2. Top is the top view of the splat, bottom shows the cross section of the image at the location shown in the top view.

In Fig. 8, the FIB image of a YSZ splat, sprayed almost under the same condition as Fig. 7, is shown. As can be seen from the image, the shape of the splat is also square. Also as can be seen from the close up image, most of the cavities between posts are filled in the middle, whereas, close to the boundaries of the splat, the cavities are partially empty.

As will be shown in the next section, the non-circular shape of the splat and its orientation (in this case, the splat's square edges are parallel to the rows of the posts) could be determined by the solidification parameters.

Effect of Solidification on the Splat Shape

Raessi et al [1] concluded from their simulations that droplet solidification is the main mechanism responsible for changing the splat shape. In this work we ran two different simulations of zirconia droplet impact on textured silicon, with the conditions presented in Table 2, indicated by case (a) and (b).

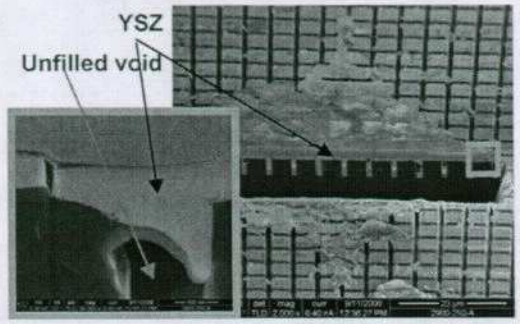
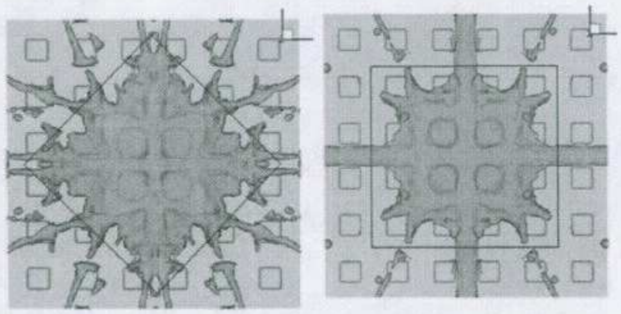


Figure 8: The focused ion Beam (FIB) image of a YSZ splat. Spaces between roughness posts filled by YSZ except near edges of splat; YSZ bridges the posts.

The conditions of case (a) and (b) are almost the same with two major differences. The initial temperature of the droplet in case (a) is 200 degrees less that the droplet in case (b). Also the thermal contact resistance used in simulations of case (a) is one order of magnitude higher than case (b). By decreasing the thermal contact resistance, the rate of heat transfer between the substrate and the splat in increased causing a more rapid solidification of the splat on the surface. In Fig. 9a, and Fig. 9b, the simulation results for two cases of (a) and (b) are shown. The major difference that is quite obvious from the result is the difference between the orientations of the splats in two cases. In case (a), where the solidification is not considered to be rapid as case (b), the position of the splat and the pattern of the substrate are diagonal with respect to each other, whereas, in case (b), the splat orientation and the surface pattern are in the same direction.



(a) **(b)**

Figure 9: Simulation results for two zirconia splats. The impact conditions are shown in Table 2.

This phenomenon can also be seen from the SEM images of the actual molten Zirconia droplets. In Fig. 10, the SEM images of zirconia splats on to two different patterned surfaces are shown. The conditions of impacts are the same and as those stated for simulations of Fig. 9 (Table 2, cases "a" and "b"). Although the impact conditions for two droplets are the same, but the different spaces between the posts will affect the fluid movement as well as the thermal contact resistance between the substrate and the drop material. (By comparing the impact conditions of nickel droplets onto two different patterned surfaces, increasing the space between the posts can decrease the thermal contact resistance, see Table 1)

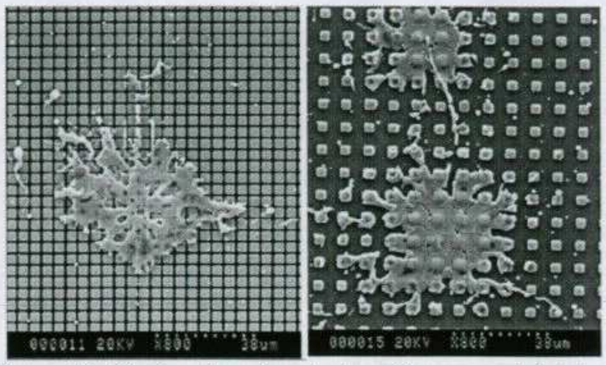


Figure 10: Single splats deposited on Si patterned: height 3.3 μm and spacing 1 μm (left) and 5μm (right) at room temperature. Particles' temperature and velocity are 2900 ºC and 250 m/s, respectively.

Effect of Surface Roughness on Porosity of the Coating

One of the objectives of this study was to understand and also to characterize the effect of the substrate roughness parameters on the creation of the pores in the coating layers in thermal spray coating. As can be seen from the numerical simulations which were also confirmed by most of the experimental results, the cavities of about 3 μm height on the surface will not completely be filled with the drop material around the edges of the splats. This means that a percentage of pores in the coating layers close to the substrate may be caused by the existence of a rough substrate. Moreover the splashing around the splats and satellite droplets will create more rough areas that in turn create more porosity on the toping layers.

Conclusion

It was shown that the developed code is able to predict the dynamic behavior of the droplet impact on the patterned surface. We showed that the numerical simulation is a great tool for investigating the effect of different parameters on the impact dynamic and solidification of the droplets.

It seems that numerical simulation of single droplet impact on the well defined patterned surface can be used to characterize the pores' sizes and locations in the coating layers that are resulting from unfilled cavities. The characterization would be based on the initial drop and the impact conditions, as well as the roughness parameters of the surface.

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