

Modeling and Experimental Validation of Deformation of Al-33Cu Droplet during Impingement on a Substrate

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Abstract Impingement of a molten Al-33Cu droplet over a substrate causes formation of a splat after spreading and solidification. Modeling of the heat transfer and fluid flow during the impingement and solidification of metal droplets on a substrate is helpful for the better understanding and control of related spray casting and thermal spray coating processes. Authors have thus developed a comprehensive mathematical model of the droplet impingement on the FLUENT 6.3.16 platform. The model takes into account all the inter-related phenomena, viz., (a) heat transfer through the droplet, solid substrate, solid-droplet interface and adjacent gaseous atmosphere, (b) fluid flow in the droplet and adjacent gas and (c) solidification. The droplet undergoes very large and rapid deformation during the impingement. The model predicts the deformation as well as the thermal and flow field within the droplet. Present work reports the experimental validation of model predictions on the droplet deformation, which was carried out using a high speed camera.

1. Introduction

The processing condition for achieving the desired splat morphology can be identified by a validated comprehensive mathematical model that predicts the flow and the thermal fields during the droplet deposition. However, due to interaction of several complex phenomena, comprehensive modeling of the droplet deposition is a challenging task. Further, the validation of the model is complicated due to the small size of the droplet as well as due to rapid deformation and cooling involved.

Mathematical models of liquid metal impingement on cold substrate have been developed to predict the deformation of impinging droplet and solidification within it. Using numerical models and experiments, Zhao et al. [1, 2] studied heat transfer and fluid dynamics during collision of a liquid droplet on a substrate. They extended the earlier model of Fukai et al. [3] to account for the relevant convection and conduction heat transfer phenomena, both in the droplet and in the substrate, in the case, when there is no solidification. Their results, therefore, are applicable to the pre-solidification stage of the impact process. Liu et al. [4] used a one-dimensional solidification model in conjunction with a two-phase flow continuum technique to track the moving liquid-solid boundary. The model, however, does not account for the convection in the liquid and conduction in the substrate. Different investigators studied the droplet deposition based on thermal resistance and temperature profile using different commercial software [5-16].

The present authors [17,24] had developed a comprehensive mathematical model that incorporates fluid flow in droplet as well as adjacent gas, heat transfer in the droplet-substrate interface and solidification. The thermal fields predicted by the models were experimentally validated using



Jackson-Hunt relationship. The present study reports the experimental validation of predictions on the rapid deformation of droplet using a high speed camera.

2. Mathematical Modeling of Droplet Impingement

Present study aims at developing a mathematical model of flow and heat transfer in a liquid metal which falls freely through gaseous medium and impinges on a cold substrate. Modeling of the phenomena is complex because it involves interactions among three phases, viz., liquid metal, solid substrate and gaseous medium. Further, as the droplet falls under the action of gravity and impinges on the substrate, its shape changes rapidly with time and its cooling is accompanied by solidification.

Figure 1 is a schematic of the impingement phenomenon. With a symmetric boundary in the middle only half of the domain (ABFCDEA) was actually computed and a very fine grid was used for the regions where impact, spreading and solidification occur. The grid for computation was finalized by grid independent test.

A droplet of Al-33wt%Cu (hereafter referred to as Al-33Cu), which is initially spherical, falls through the gaseous medium and impinges on a grade 304 stainless steel substrate. At the droplet/substrate interface a gap was created. This gap was used to model the interfacial contact resistance by prescribing an effective thermal conductivity to the gap. The thickness of the substrate was assumed to be 1mm. Since the initial shape of the droplet is assumed to be spherical, the fluid flow and the heat transfer are axisymmetric (r-z direction).

The following assumptions have been made in the mathematical model:

1. Droplet is initially having spherical geometry and it remains so just before the impingement.
2. The problem is axi-symmetric about the axis shown in Figure 1.
3. Velocity of the droplet impingement is perpendicular to the plane of the substrate and no rotation of droplet occurs along the axis.
4. The flow of metal Al-33Cu droplet and gas is laminar and incompressible. The velocity of gaseous media at domain walls is zero.
5. Walls of the domain (Figure 1) are assumed to be at 300 K.
6. The heat transfer is dominated by conduction and convection modes. Therefore, radiation is ignored.
7. To take into account the thermal contact resistance due to air gap a solid layer has been defined. The conductivity of the solid layer was assigned by a constant value.
8. Initial velocity of droplet (when it forms) is zero. It acquires velocity during the free fall. The

velocity just before the impingement was $\sqrt{2gH}$, where H is the distance between the orifice of crucible and substrate. The other important information on the mathematical model like the governing equations and discretization method have been described elsewhere [20,28].

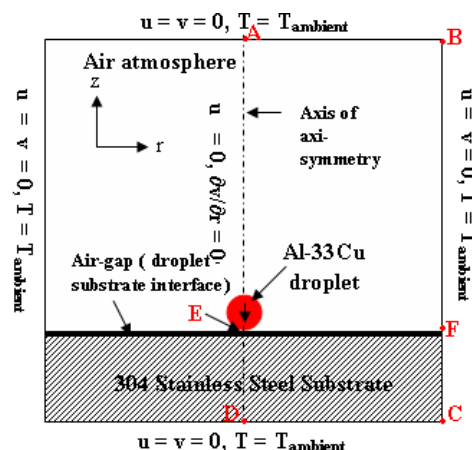


Figure 1. Schematic Representation of the Mathematical Model of Droplet Impingement.

All zones were initialized with the temperature of 300K, except the droplets. The droplets were set to a predetermined higher temperature. The initial velocities at every point inside the domain were zero, except within the droplets.

Since problem is axis-symmetric only half of the domain shown in Figure 1 was considered in the computation domain. Axis of symmetry was like a free-slip wall. The normal velocity was zero. Tangential velocity did not have normal gradient. Thus along the axis of axis-symmetry $u = 0$ and $\partial v / \partial r = 0$. At the other boundaries $u = 0$ and $v = 0$. Since these boundaries are far away from the droplet, the temperatures at these boundaries were set equal to the ambient temperature, i.e., 300 K. The above described model was simulated using FLUENT 6.3.16 plat form.

Thermo- physical properties of Al-33Cu and 304 stainless that have been used for simulation are taken from ref. [20]. The thermal contact resistance $7 \times 10^{-4} \text{ m}^2 \text{ Kw}^{-1}$ at the interface of Al-33Cu droplet and the grade 304 stainless steel substrate was taken from the work of Kumar et al [20].

3. Experiments for Validation of model

A droplet impingement set up to validate the model was fabricated. Figure 2 shows the schematic sketch of the set-up. A vertical resistance furnace was used for melting. The furnace has a cylindrical shape having a height of 8 inch, an outer diameter of 4 inch and an inner diameter of 1 inch. The furnace was capable of rapid heating of the charge. The temperature of the melt could be controlled within $\pm 5^\circ\text{C}$. It was placed at the top of the droplet impingement chamber as shown in Figure 3. A quartz tube with an inner diameter of 17 mm was used as a crucible. At the bottom of the crucible there was a melt delivery nozzle. The diameter of the melt delivery nozzle was 2 mm. The inner wall of the quartz was coated with alcohol shoot, which suppressed the reaction between molten metal and quartz tube. Substrate was made of grade 304 stainless steel. The substrate was circular in shape having a diameter of 20 cm and thickness of 20 mm. It was placed inside the spray chamber. It was placed on a threaded stand, such that it could be moved up and down. Pieces of master alloy Al-33Cu were melted in the quartz crucible. The temperature of the melt was maintained at $\sim 150^\circ\text{C}$ above the melting point. For each droplet impingement experiment, 50 gram charge of the alloy was charged into the crucible where the temperature was 700°C . The temperature of the melt was monitored by a thermocouple inserted between the quartz crucible and the furnace inner wall. By application of air pressure droplets were pushed out of the 2 mm diameter melt delivery nozzle. These droplets impacted on the substrate, deformed and finally solidified on it. For deposited splats, the size of the droplet was estimated by measuring the size of splats.

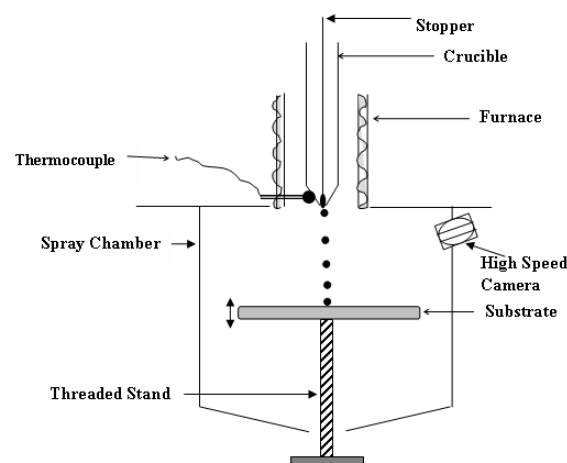


Figure 2. Schematic Sketch of Droplet Impingement Set up

4. Results and Discussions

In the present work the mathematical model of the droplet impingement assumes a thin layer of air – gap in between the impinging Al-33wt%Cu (Al-33Cu) droplet and the stainless steel substrate (Figure

1). $7 \times 10^{-4} \text{ m}^2 \text{ KW}^{-1}$ was taken as the value of the thermal contact resistance and $1.43 \text{ Wm}^{-2} \text{ K}^{-1}$ as the value of the conductivity of the interface air-gap layer in the droplet impingement model (Shown in Figure 1).

5. I. Deformation of Al-33Cu Droplet

Numerical simulations and experiments were carried out for the impingement of Al-33wt%Cu droplets on the grade 304 stainless steel substrate. In the current study simulation and experimental studies were performed for shape evaluation of impinging molten 6.2 mm diameter droplet with velocity 3.13 m/s on to the stainless steel substrate.

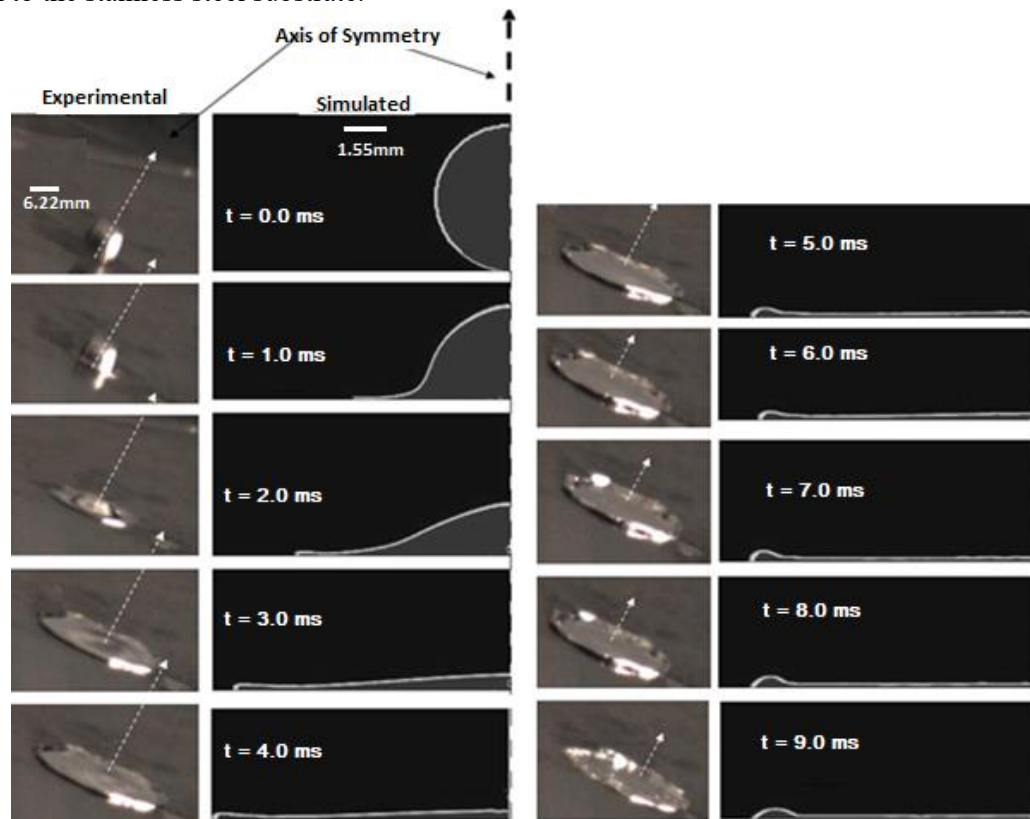


Figure 3. Comparisons of Photographs and Simulated Images a 6.2 mm Diameter Al-33Cu droplet.

At the moment of impingement, the high impingement velocity creates a high pressure region under the droplet and forced the liquid metal to flow over the contact surface while the effect of surface tension was comparatively less; the maximum flow velocity was achieved at the edge where all the momentum was transferred to the radial direction, and the cross-section area was small. The sequence of deforming droplet was recorded using a high speed camera (FASTCAM- Super 10 KC, Photron USA, San Diego, CA), which can capture the photographs at the speed of 1000 frame per seconds. Figure 3 presents the result of simulation of impingement of a Al-33 Cu droplet having a diameter of 6.2 mm and compares the computed shape of the droplet for different durations of time after the droplet comes in contact with substrate, with that recorded by high speed video camera. It is clear that the simulated Al-33wt%Cu droplet profile is in good agreement with that from the experiment as shown in the Figure 3. The forces which cause the deformation of droplets are gravitational force and the force due to high velocity of impingement. The forces due to viscosity and surface tension oppose the flow of molten metal. Droplet spreads radially after impingement on the substrate along the surface of the substrate as shown in the Figure 3. With the spreading and solidification progressed, the flow of liquid metal reduced and the effect of surface tension became significant, which generated high pressure regions at the edges and finally reversed the flow back

towards the centre as shown in the 4.0 ms time frame plot in Figure 3. This resulted into the formation of bump at the edge of the splat. When a solidification layer grows, the lower part of the liquid splat loses momentum as it solidifies to become a part of solidified layer. Solidification may take place during spreading, but the solidified layer growth velocity is slow compared to when solidification starts after complete spread. Therefore, a splat retains radial momentum during spreading and reaches its maximum diameter while solidifying. The simulated evolution of droplet shape has been reported earlier paper [8]. The bump near the edge has been observed even when there is no cooling [22]. The physical reasons for the bump formation are not fully understood although surface tension and the existence of the bump because of the maximum cooling near the edge (Figure 3) [8] could be suggested as two of the reasons. The shape of the splat remains same after 9.0 ms till the complete solidification. Droplet becomes solid after 67.7ms. The solidification of droplet starts from the periphery of the splat because outer edge of the droplet remains in continuous colder part of the substrate, which causes faster heat transfer.

The evolution of the shape of liquid droplet impinging a solid substrate is a complex phenomenon. However, this has been studied by many investigators [8, 22-25]. An important parameter which decides upon the evolution of shape of the liquid droplet is Weber number, i.e., density, viscosity, impingement velocity and surface tension. Depending on the Weber number different types of shape evolution are possible. In numerical method the shape of the splat depends on contact angle, cooling and solidification characteristics. Cooling and solidification characteristics of molten metal depend on thermal contact resistance between molten droplet and the substrate. The value of contact angle for which simulation results were in good agreement with experimental results was 58° , although simulations have been carried out for different value of contact angle and found different morphologies of the splat.

They have calculated by inverse method between the grade 304 stainless steel and molten Al-33wt%Cu. In experiment droplet impinged the substrate normally, but due to inclined camera arrangement in the set up, the droplet appears to be hitting the substrate at some angle or the substrate appears to have some inclination with horizontal as shown in the Figure 3. In fact substrate was horizontal and direction of droplet impingement was perpendicular to the substrate.

The sequence of impingement as shown in the Figure 3 shows that the droplet deforms on to the substrate into the shape of a cap and cone shape with flat edge symmetric around the axis of symmetry up to 2.0ms followed by formation of bump at the periphery of the impacting droplet after 3.0ms. Theoretical predictions [20, 28] have shown that a molten Al-33wt%Cu droplet impacting on a 304 stainless steel substrate starts freezing first at the outer most edge, where the substrate temperature is lowest. Therefore, solidification restricts the further spread of the splat and surface tension becomes predominant at the lower temperature and tries to pull back the liquid metal inwards. Therefore there is formation of bump at the periphery of the splat as shown in the Figure 3. Therefore, the final shape of solidified splat is like a circular disc as obtained. As shown in Figure 3 the numerical results are in qualitative as well as quantitative agreement with the experiments. So, it is one of the way in which the impingement model can be validated is by comparing the simulated deformation of droplet with the video photographed image. The same has been reported in this study. Figure 3 shows the actual deformation of a droplet having diameter of 6.2 mm (photographed using high speed video camera) along with the simulated deformation. The initial temperature of the droplet was 973 K and the velocity of impingement was 3.13 ms^{-1} .

6. Conclusion

In the present study, the impingement of a molten metal droplet (Al-33wt%Cu) is simulated using a commercial computational fluid dynamics software, FLUENT 6.3.16, in which a two dimensional axis-symmetric domain for deformation considering the free surface deformation and solidification have been developed by using the VOF technique with a enthalpy porosity method. The VOF technique in combination with solidification model was used to simulate the impingement of Al-

33wt%Cu droplets on the 304 stainless steel substrate. The model was validated by comparing the predictions with experimental data. The outcomes of the present investigation are listed below.

1. Fluent 6.3.16, finite volume method based code has the capability of obtaining a convergent solution of the equations established in simulation of impingement of a molten droplet impacted at a high velocity.

2. The deformation behavior of the droplet was characterized by the spreading and evolution of shape of the splat, the predicted results were in good match with the experimental.

3. A comprehensive model has been developed that accounts the effect of surface tension as well as solidification.

4. Model can predict the formation of bumps accurately during droplet deposition based processes.

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