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Numerical study of molten and semi-molten ceramic impingement by using coupled Eulerian and Lagrangian method

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Abstract—Large temperature gradients are present within ceramic powder particles during plasma spray deposition due to their low thermal conductivity. The particles often impinge at the substrate in a semi-molten form which in turn substantially affects the final characteristics of the coating being formed. This study is dedicated to a novel modeling approach of a coupled Eulerian and Lagrangian (CEL) method for both fully molten and semi-molten droplet impingement processes. The simulation provides an insight to the deformation mechanism of the solid core YSZ and illustrates the freezing-induced break-up and spreading at the splat periphery. A 30 μm fully molten YSZ particle and an 80 μm semi-molten YSZ particle with different core sizes and initial velocity ranging from 100 to 240 m/s were examined. The flattened degree for both cases were obtained and compared with experimental and analytical data.

Keywords: Thermal spray; Semi-molten particles; Coupled Eulerian and Lagrangian method; Flattening degree

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1. Introduction

Thermal spray technology encompasses several processes which are used to create performance enhancing coatings. The coatings are formed by heating and accelerating micro-sized and nano-sized particles toward a targeted substrate surface. These particles initially impact onto the substrate where they deform and adhere. The particles then impinge onto one another, building up the coating particle by particle in a lamellar structure. The degree of deformation of these particles and their adhesion strength at the substrate can be attributed to several factors, including: particle impact velocity, particle size, particle melt fraction, particle material properties, wetting of the substrate by molten particles, temperature of the substrate and substrate roughness.

With the development of smarter and more complex oxide ceramic film applications, such as the dye-sensitized solar cell and functionally graded bioactive coatings, a detailed understanding of the deposition process at the substrate is required in order to control the adhesion, cohesion and porosity of the coatings. By coupling the jet and particulate phases, numerical models are capable of simulating the transient velocity, temperature and phase content of the powders traveling through a thermal spray device. The thermal-physical state of an individual particle can therefore be predicted at the substrate surface which can then be relayed into a focused impingement model in order to simulate the impingement and buildup of the coating microstructure particle by particle. The most developed finite element simulations for unmelted, solid particle impingements can be found in [1,2] for copper powder deposited by cold spray, and in [3,4] for tungsten–carbide cobalt (WC–Co) powder deposited by HVOF combustion spray. By utilizing the Johnson–Cook strain hardening, temperature softening plasticity model, the deformation and stress of the solid metal particles could be captured. However, thermal plasma spray is commonly utilized to deposit oxide ceramics such as YSZ in the size range of 20–90 μm [5,6]. Depending on the initial size of the coating powder, some particles hit the substrate at a fully molten state. Meanwhile other particles larger than 60 μm [7], are partially molten with a solid core due to high plasma gas temperature and high temperature gradient of particles caused by the low thermal conductivity of ceramic powders.

Despite lack of detailed understanding for the deposition of semi-molten droplet impingement, little modeling and simulation work has been reported, given the challenges of solving both solid and liquid phases simultaneously. The rule-based approach in [8] presents an efficient and unique way of estimating the porosity created during the

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coating buildup of molten and semi-molten droplets. However, this method is not able to capture the detailed physics during the particle impingement process. The works presented in [9] and [10] are limited to 2D simulations, without details such as substrate heat transfer and solidification respectively, which are crucial elements in determining the splat morphology. Furthermore, a central core is not modeled as a moving solid in both cases. In a more comprehensive work by Tabbara et al. [11] a semi-molten ceramic droplet with a moving solid core was simulated at a relatively low velocity. A temperature gradient within the particle was predefined and the whole deformation of the liquid shell was captured accurately in consort with the freezing-induced break-up mechanism at the splat periphery. Alavi et al. [12] considered the influence of phase change after the impact in conjunction with the influence of the core size on impact dynamics. Wu et al. [13] expanded the validity of the aforementioned models for higher impact velocities between 100 to 200 m/s. In all previous studies listed above, the Volume of the Fluid (VOF) approach was utilized assuming that the solid core behaves as a rigid body without considering possible deformation of the solid core and the substrate at impact.

According to Li et al. [14], brittle materials may possess ductile behavior under particular conditions such as very high temperature or high pressure. In this case, modeling the solid core as a rigid body may produce unrealistic results. Therefore, new approaches are required for simulating both the liquid and the solid part simultaneously in a coupled manner. This investigation is the first of its kind, to simulate a semi-molten droplet impingement using a coupled Eulerian and Lagrangian (CEL) approach for thermal spray applications. The 3-D study particularly examines the splash deposit of the liquid ceramic shell, and the deformation of the solid core and substrate. The results give an insight of the morphology of fully molten ceramic particle impact and illustrate how semi-molten ceramic particles behave under dynamic impact conditions. The flattening degree of the particles are obtained and compared with both experimental and analytical data.

2. Numerical method

In the first case of fully molten YSZ particle, a 30 μm particle, with an initial velocity of 190 m/s was generated based on real spray parameters provided by Vardelle et al. [5]. Owing to the axisymmetric nature of the normal impact process, only a quarter of the computational domain was simulated as shown in Fig. 1(a). The particle impacting velocity was increased progressively from 100 to 240 m/s and the flattening degree for each case was obtained. The second case of semi-molten particles was simulated based on the experimental findings provided by [7]. The particle diameter was set to 80 μm with several solid core diameters. Due to the low thermal conductivity of the YSZ material, a temperature gradient along the radius of the sphere particle develops during thermal spraying [11,15]. The liquid outer shell was assigned an initial temperature gradient as shown in Fig. 2. The temperature profile within the solid core and toward the center was assumed constant based on the particle temperature profile provided in our previous studies [11,15].

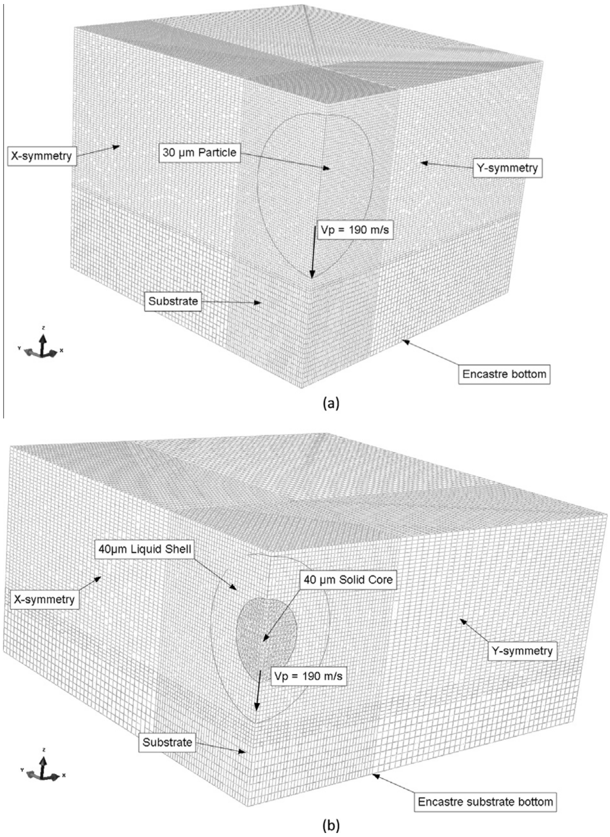

Fig. 1. (a) Computational model of molten particle impact benchmark. (b) Computational model of semi-molten particle impact with a core diameter of 60 μm.

The computational domain and mesh of semi-molten particle is illustrated in Fig. 1(b). In the explicit analysis, the stable time increment Δt_{stable} is given by:

$$\Delta t_{stable} < \frac{L_e}{C_d}$$

where L_e is the smallest element dimension and C_d is the wave speed in the material. The requirement for a fine mesh with small elements to capture the detailed physics of the process leads to very short maximum allowable time increments which, in turn, result in a computationally intensive analysis. In order to optimize the computational efficiency of the impact model, smaller elements were used only in the particle and along the particle–substrate interface. A mesh convergence study was carried out by varying the mesh density in the particle and along the contact interface. The mesh and geometry were generated using FEA software Abaqus/Explicit [16]. Given the velocity, viscosity, as well as characteristic length varying from case to case, the Reynolds Number in this paper will vary from 500 to 3000. The details of the mesh and solver could be found in Table 1.

2.1. Impingement model

The method for modeling the liquidus YSZ, Stainless Steel substrate, temperature profile, thermal and flow models is outlined below. The thermal-physical properties of the materials presented in this paper are summarized in Table 1.