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Modeling YSZ droplet impact with solidification microstructure formation under a horizontal electric field in plasma spraying

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Abstract

Current numerical models simplify the solidification microstructure formation process in plasma spraying conditions, and deal little with droplet shape control while undergoing solidification microstructure formation via external forces. The paper may shed light on how to control splat shape and crystal growth in plasma spraying by developing a novel model. Centered on the Cahn-Hilliard equation, the current numerical model employs the coupled Navier-Stokes equations to track the liquid-gas interface, and by virtue of an embedded phase field model combined with the heat balance equation, captures grain-grain boundary and solid-liquid interface. The electric force is added as a source term in the Navier-Stokes equations and the fluids are assumed perfect dielectrics. Explicit finite difference solutions are sought with the aid of parallel computing. The major findings are that the electric force exerts little effect on microstructure formation but changes dramatically drop shape and hence solidification time. Besides, the recoiling could be prevented completely, resulting in a pancake like splat of reduced thickness.

Keywords: phase field method, polycrystal growth, Cahn-Hilliard equation, multiphase flow

1 Introduction

Owing to the expensive plasma spraying equipment and difficulties in carrying out experiments for single droplet impact in plasma spraying conditions, many numerical studies have been done. Zhang et al. [1] conducted YSZ droplet impact that was undergoing solidification on an incline using the smoothed particle hydrodynamics (SPH) method. The impact was 2D and the authors ascribed the enlarged spread factor to the simplification of the 2D model. Utilizing the SPH method, Ma et al. [2] proposed a new criterion for splash of both heavy and light drops. They also analyzed the criteria for heavy and light drops, finding that the incident kinetic energy is key to determining the outcome of heavy drop impact. Employing the Cahn-Hilliard based phase field method, Shen et al. [3] probed into the dynamics of supersonic YSZ droplet impact in practical plasma spraying conditions. They observed that the solidifying time for an YSZ droplet of diameter around 10 μm is typically less than 1 μs. Wu et al. [4] studied partially molten YSZ impact under practical conditions. The findings are that, when the solid core is small compared with the particle diameter, the impact is similar to that of a fully molten droplet. Nevertheless, splashing takes place as the solid core gets larger. As for the effect of the trapped air in hollow Zirconia droplets, Safaei et al. [5] via simulations concluded that when the velocities exceed 100 m/s the trapped air contributes much to droplet splashing. Undercooling isn't accounted for in the above studies. However, it is crucial for crystal growth and the duration of solidification. Via the Volume of Fluid method, Shukla et al. [6] examined the spreading of a molten Zirconia droplet with nucleation undercooling, observing that larger nucleation undercooling would lead to a relatively lower interface temperature and a higher interface velocity.

Having surveyed the literature, it is found that little effort, to the best knowledge of the authors, has been exerted on the study of droplet impact with solidification microstructure formation under a horizontal electric field in plasma spraying conditions, while investigating this may provide better insight into droplet shape control and into crystal growth under an electric field. Therefore, the paper aims to develop a comprehensive numerical model to predict droplet impact dynamics with microstructure formation under a horizontal electric field.

2 Methods

Since the governing equations, except the one for the electric field, have been described in detail in [7], they would be summarized here. The readers are referred to [7] for details. To study drop impact under electric force, an extra external force, represented by $\nabla \cdot \boldsymbol{\tau}^M = -\varepsilon_0 E^2 \nabla \varepsilon_r(c)/2$, has been added in the Navier-Stokes equation. Eq. (5) is to compute the evolution of the potential ψ. The fluids are assumed perfect dielectrics.

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho(c)\frac{D\mathbf{u}}{Dt} = \nabla \cdot \mathbf{T} + \rho(c)\mathbf{g} + G\nabla c + \nabla \cdot \boldsymbol{\tau}^M + \mathbf{S} \tag{2}$$

$$\rho(c)c_P(c)\frac{DT}{Dt} = \nabla \cdot [k(c)\nabla T] + \frac{\rho_l L_l}{2}\frac{\partial \phi}{\partial t} \tag{3}$$

$$\frac{Dc}{Dt} = M\nabla^2 G \tag{4}$$

$$\nabla \cdot (\varepsilon(c)\nabla \psi) = 0 \tag{5}$$

$$\tau_\phi \frac{\partial \phi}{\partial t} = [\phi - \lambda u(1-\phi^2)](1-\phi^2) + \nabla \cdot (\mathbf{\Lambda} \cdot \nabla \phi)$$
$$-2s(1+\phi)|\nabla\theta| - \varepsilon_\theta^2(1+\phi)|\nabla\theta|^2 \tag{6}$$
$$\tau_\theta(1+\phi)^2 P(\varepsilon_\theta|\nabla\theta|)\frac{\partial \theta}{\partial t} = \nabla \cdot \left[(1+\phi)^2\left(\frac{s}{|\nabla\theta|} + \varepsilon_\theta^2\right)\nabla\theta\right] \tag{7}$$

The boundary conditions are given in Fig. 1. First, for computation of the electric potential ψ, fixed values are set on the left and right borders. Second, χ contains all field variables, except for all the velocity components on the wall, for the normal velocity component on the axis of symmetry, and for the order parameter c on the substrate surface that satisfies $\xi\gamma\alpha\mathbf{n} \cdot \nabla c + f_w'(c) = 0$, where $f_w(c)$ is the wall free energy density and $\mathbf{n}$ is the unit normal outwards.

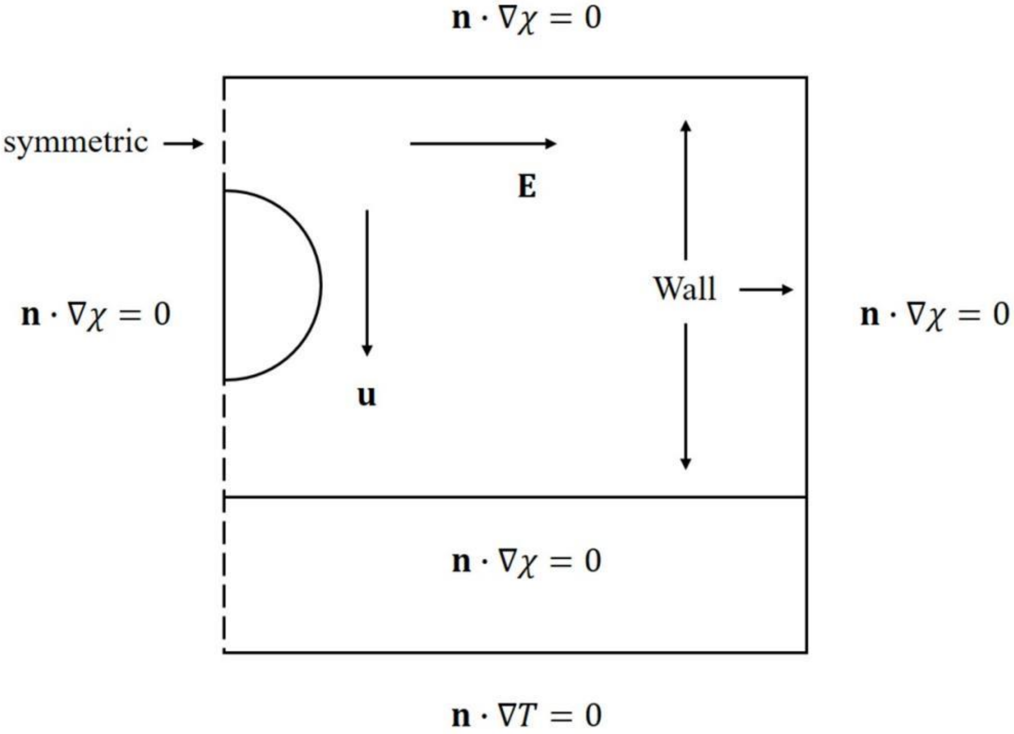


Figure 1: Schematic of the problem with boundary conditions defined.

The set of equations are explicitly discretized using the finite difference method, with upwind scheme to deal with convective terms. The flow equation is solved via the popular projection method. Parallel programming based on OpenMP is applied.

3 Results

This section focuses on a molten YSZ droplet impact with and without a horizontal electric field. The effect of mesh size and of the phase field mobility has been carefully checked, with thermophysical properties and numerical configurations found in [7]. The impact velocity is 50 m/s, with numerical outcome presented in Fig. 2.

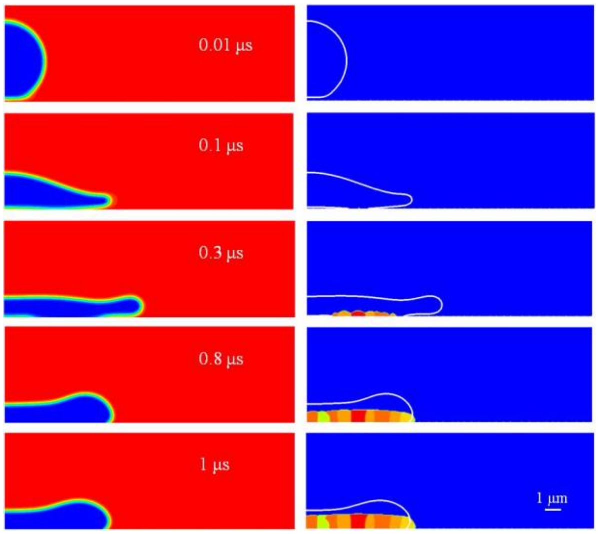


Figure 2: Droplet shape at different instants without an electric field. Left is the drop shape. In the right, the different colors represent grains of distinct orientations.

At 0.01 μs, the stagnation pressure built beneath the drop dimples its bottom, which takes on a flat shape. The bottom will eventually touch the substrate via a line contact, since a little portion of air would be trapped in the impact center. It is noted that the white iso-contour corresponds to c=0.5. The characteristic in the recoiling phase is the continuous thickening of the rim. Since the liquid in contact with the substrate has been frozen by 0.8 μs, the spreading factor remain unchanged. Besides, the crystals exhibit a columnar structure, driven by the vertical heat flux. To check the effect of electric force, a simulation was run with the electric field intensity being 2.78 MV/m. Other numerical configurations are the same. The outcome is displayed in Fig. 3.

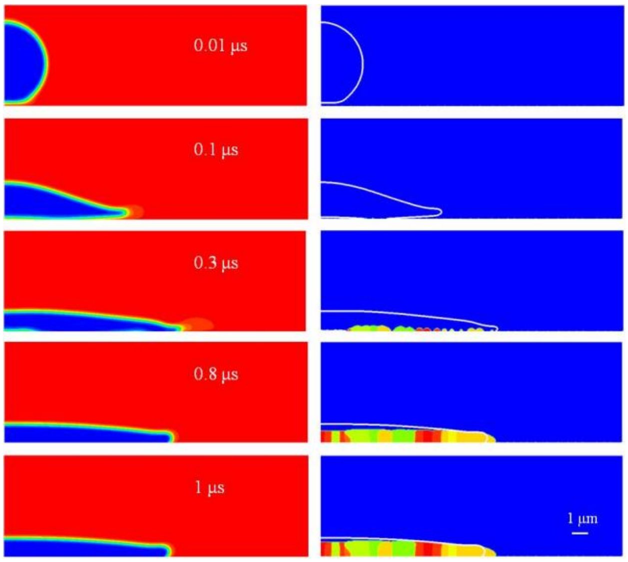
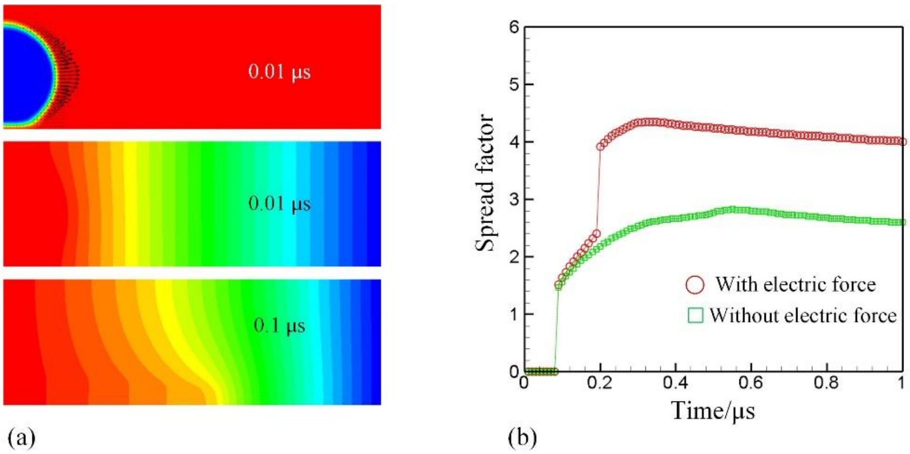


Figure 3. Droplet shape at different instants under an electric field. Left is the drop shape. In the right, the different colors represent grains of distinct orientations.

Fig. 3 exhibits a number of differences. At 0.1 μs, being visually recognizable is the sharpening of the spreading front. Under electric force, the droplet is stretched like an elastic so that the contact area between the droplet and substrate surface increases. Accordingly, more nuclei start growing as demonstrated at 0.3 μs on the right column. The droplet profile changes little after 0.3 μs and takes on a pancake shape. The columnar structure still dominates, showing that the electric force does not show evident effect on it.



(a) (b)

Figure 4: (a) Electric force and potential distribution. (b) Spread factor evolution.

Fig. 4 gives the electric force and potential distribution at particular instants. Notice that in Fig. 4 (b) the initial discontinuity is due to the releasing of drop some distance above the substrate, and that the second discontinuity in the red circle is probably caused by the rapid touch of the spreading front onto the substrate.

4 Conclusions and Contributions

Previous numerical models dealing with droplet impact with solidification often simplify the handling of solidification via the enthalpy or the like methods. Such models are not able to mimic crystal growth microscopically. Meantime, using external forces to tail splat shape in plasma spraying is rarely reported. The paper therefore presents a comprehensive model to that end. Centered on the Cahn-Hilliard equation, the current numerical model employs the coupled Navier-Stokes equations to track the liquid-gas interface, and by virtue of an embedded phase field model combined with the heat balance equation, captures grain-grain boundary and solid-liquid interface. The electric force is added as a source term in the Navier-Stokes equations and the fluids are assumed perfect dielectrics. Explicit finite difference solutions are sought with the aid of parallel computing. The major findings are that for an YSZ of diameter around 5 μm impacting at 50 m/s, the electric force exerts little effect on microstructure formation but changes dramatically drop shape and hence solidification time. The electric force stretches the droplet as if it were an elastic, resulting in an enlarged spread factor and reduced solidification time. Besides, the recoiling could be prevented completely, leading to a pancake like splat of reduced thickness.

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