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Phase-field modeling on laser melting of a metallic powder

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ABSTRACT

Laser-based manufacturing process such as selective laser melting, sintering, and direct deposition using metallic powders plays an important role in additive manufacturing technology. As spatial resolution increases, there is a great need to advance the design, quantitative analysis, and optimization of relevant thermal fluid processes at the powder level. In this paper, a theoretical model is developed to characterize melting and Marangoni flow dynamics within a pure metal powder heated by a moving Gaussian laser beam. Phase field formulation is developed to simulate the solid-liquid phase transition along with the thermocapillary effect at the free surface, which drives the molten flow within the powder and thus influences heat transfer behaviors. The formulation, simplification, and computational results for two-dimensional cases are demonstrated and discussed in detail.

1. Introduction

Selective laser melting, sintering, and deposition of metallic powders are applied in many laser-based manufacturing methods. The layer-by-layer building process plays an important role in additive manufacturing (AM) or solid freeform fabrication for the manufacture of geometrically complicated metallic parts that are difficult to make by conventional methods [1]. However, the process design, quality and reliability, and optimization are challenging issues in AM processes due to limited analysis and predictive modeling tools that can describe the physical events across multiple of temporal and spatial scales and for materials with multiple components [2–4]. In practices, thermal fluid processes in AM cover dynamics of solid, liquid, and vapor phases, interfaces between phases, and metallurgical mechanisms. The relevant fluid flow and heat transport phenomena involve thermal conduction, convection, radiation, and interfacial transport induced by a moving laser beam. The physical behaviors of typical AM processes are fully coupled across phases, and geometrically complicated around the melt pool, the thin powder layer, and the heat affected zone. Specifically, issues in selective laser melting include power, spot size and scanning speed of the focused laser beam, dynamic powder deposition, completeness of melting or sintering and resolidification of metallic powders, stability and evaporation of the molten metal, and the thermocapillary effect induced by an inhomogeneous temperature distribution at the free surface [5]. These are all relevant to the surface defects caused by incomplete melting, lapping, and/or gas entrapment during the process, and thus have significant impacts on the quality of AM manufactured parts. Although near-net-shape production is a significant advantage of AM process, the as-manufactured parts or specimen usually have rough surfaces and are subjected to early fracture in a fatigue test [6]. These surface defects, such as notches and cracks, are formed by adjacent powders that are partially melted, which may cause crack initiation and propagation and eventually results in a part failure. As the new technology and AM machines keep moving forward, theoretical studies on the multiscale events and relevant thermal processes are relatively limited. There is a great need of fundamental studies at the powder level that can better understand the underlying transport phenomena and the metallurgical mechanisms to provide quantitative information, fully optimize the process, reduce the process time and material cost, and eventually to enhance the quality of the manufactured parts.

Theoretical studies of melting and sintering induced by laser heating and the heat transfer characteristics across a powder bed can be found in a few investigations by Zhang et al. [7–9]. Specifically for the development of AM technology, Ladani et al. have analyzed the temperature distribution and melt pool configuration as well as the effective thermal conductivity and capillarity effects during a powder bed fusion process for various materials including Ti64, Inconel 718, stainless steel, and aluminum powders [10–12]. In stead of a powder bed, in this paper we focus on the analysis on small scale and discrete powder level by considering single powder

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melting and Marangoni flow dynamics of pure metal processed by a focused laser beam. The conceptual investigation at the single-powder level is helpful to understand challenging problems such as selective laser melting or sintering process that involves powder-powder or powder-substrate interaction, interfacial instability, and collective behaviors of powders. The governing system is formulated based on the phase field or smooth interface method. This approach has advantages in accommodating interfacial dynamics and phase transition kinetics including melting, solidification, and fluid flow. Phase field variables are considered in the transport phenomena, which naturally incorporate the moving boundary or interfaces into the phase field function(s). In the phase field approach, the concept of gradient energy was first introduced by van der Waals [13] in describing gas-liquid phase transition with a diffuse interface across liquid and vapor phases. Cahn and Hilliard [14] described the non-equilibrium phase transition at solid-liquid interface using a phase field variable, which is uniform in solid or liquid state but has a narrow and smooth transition profile across the interface. The phase transition is driven by the reduction of the free energy, specifically, the gradient energy due to spatial variation of density or concentration [14]. As a result, the continuous phase field equation that governs the local state of the material can clearly distinguish the location of the transition interface between liquid and solid domains. Similarly, the general approach applied to the dynamic behaviors of fluid systems near critical state can be described by the Model H [15]. Other than Cahn-Hilliard model and Model H, an alternative way to derive the phase field formulation is known as the entropy approach, in which the entropy property is the starting point of derivation to accommodate the gradient effect. The thermodynamic framework was developed by Penrose [16], Kobayashi [17], and Wang [18] et al. Wang discussed the definition and constrains for defining the smooth transition function between two phases. Anderson [19,20] and many others [21–23] extended the method to multi-component and multi-phase problems with and without convective effect. The solid-liquid phase-transition kinetics for a sharp-interface is associated with the Gibbs-Thompson effect [24], which provides a theoretical estimation of the interfacial mobility, important in determining fast solidification and dendritic growth process [22]. A relevant diffusion-based solid-state sintering process studied by phase field method was proposed by Wang [25]. A summary of recent progress of the phase field method in multiphase flow modeling can be found in an excellent review by Lamorgese et al. [26].

Here we apply the entropy approach to derive the governing equations for the problem in hand. A pure metal powder particle with diameter about tens of microns is heated by a moving Gaussian laser beam with small spot size approximately the powder diameter. The phase transition kinetics is considered relatively fast to a degree that the process is controlled by thermal transport. We focus on the coupling of powder melting and thermocapillary dynamics. The substrate cooling and gas phase transport are neglected. The temperature-dependent material properties including thermal conductivity, interfacial energy, and the melt viscosity are considered in our formulation. The computational results on the transient dynamics of the fluid flow and heat transfer are demonstrated and discussed in detail.

2. Theoretical analysis

Fig. 1 shows the schematic view of the conceptual model. A few assumptions are proposed to simplify the theoretical analysis: (i) the small deformation of the free surface is assumed negligible due to small powder size and relatively strong surface tension for metals, (ii) the solid-liquid interfacial energy is difficult to obtain for a metallic system, and thus here we assume that its magnitude is about half of the surface energy at the liquid-vacuum interface, (iii) evaporation of the liquid metal and the influence of the gas phase, including the participation of gas content in radiation heat transfer, are all neglected, (iv) the powder is suspended in a vacuum space without substrate cooling, and (v) thermal expansion and thermal stress, elasticity, and the blowing velocity at the melting interface due to density variation are all neglected as density is assumed constant for both liquid and solid phases. The moving Gaussian laser beam is focused down to a range of approximately the size of the powder. The temperature-dependent material properties in this study include interfacial energy, thermal conductivity in the solid phase, and dynamic viscosity of the molten metal. Furthermore, the specific heat, density, and the latent heat are assumed constants. The moving melting interface is isotropic and assumed thermal transport-controlled instead of kinetics-controlled. The assumptions listed above are applicable to many-powder interactions except item (i), where the spherical approximation is no longer relevant to deformable interfacial dynamics due to powder-powder interactions.

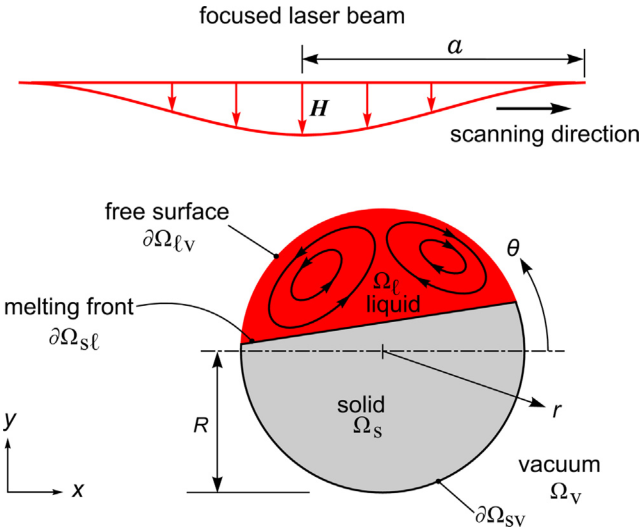

Fig. 1. Schematic of the conceptual model showing the physical domains of a melting powder and the thermocapillary effect due to spot laser heating. The gray area indicates solid phase, while the red area is the molten metal with circulations induced by thermocapillarity. The solid-liquid interface is determined by the isoline of zero phase field. The simplified outer domain is presumable a vacuum space. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2.1. Phase field formulation

The conduction, convection, and simplified thermal radiation heat transfer all play significant roles in the powder melting process. We summarize the governing equations for a general compressible substance, and then apply a quasi-incompressible assumption to simplify the formulation. The arbitrary melting interface can be determined by the phase field equation, derived based on the entropy approach [18–20]. By taking gradient effect into account, the entropy functional of the system $\mathcal{S}$ is contributed by the entropy density in the homogeneous bulk phase and the spatial variation of the phase field function ϕ over the material volume Ω, expressed as

$$\mathcal{S} = \int_\Omega \left[\rho s(e, \phi, \rho) - \frac{1}{2}\xi_s^2 |\nabla\phi|^2 \right] dV, \qquad (1)$$