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Surface-active element transport and its effect on liquid metal flow in laser-assisted additive manufacturing

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A B S T R A C T

During laser-assisted additive manufacturing, the transport phenomena, solidification behavior, and melt pool geometry are affected by base-metal sulfur content and oxygen present in the atmosphere. The role of these surface-active elements during metal-based additive manufacturing is not well understood. In this study, the mass transport of sulfur and its effect on liquid metal convection (Marangoni flow) are examined by using an improved 3D transient heat transfer and fluid flow numerical model. An improved surface tension model is proposed to take into account the influence of sulfur content and temperature at the surface of melt pool. The sulfur mass transport equation is combined with the other conservation equations. The results show that the sulfur redistribution leads to transitional Marangoni flow. The powder addition into the melt pool results in the dilution of sulfur in the melt pool. Increase in mass flow rate and energy input results in decreased temperature coefficient of surface tension. When temperature coefficient of surface tension changes sign from positive to negative, the flow motion transition from inward flow to outward flow occurs. Two predominant types of flow pattern lead to two types of fusion boundaries of deposited track.

1. Introduction

In laser-assisted additive manufacturing, a deposited layer is obtained through melting metal powder delivered and deposited on the surface of the base metal. Many complicated physical phenomena, such as laser-powder interactions, heat and mass transfer, fluid flow, melting, and solidification are involved in this process [1–3]. Since the Peclet number is on the order of 10^2–10^5 in the melt pool in laser-assisted additive manufacturing, convection plays a vital role in the heat transport and the melt pool formation [4]. The convection in the melt pool is driven by various driving forces. Marangoni stress has been proven to be the main driving force [5,6]. Owing to the spatial gradient of surface tension driven by the temperature or compositional gradients, the Marangoni stress arises on the melt pool surface [7]. The Marangoni stress is defined by the spatial temperature gradient multiply by the temperature coefficient of surface tension on the surface of melt pool.

The content of surface-active elements of group VIA (i.e. oxygen, sulfur, selenium, and bismuth) in the melt pool has an influence on the direction and magnitude of Marangoni stress [8,9]. If surface-active elements are not present in the melt pool, the temperature coefficient of surface tension is negative, and liquid metal flows outwards along the surface of melt pool [8]. If surface-active elements are present in the melt pool, the temperature coefficient of surface tension may become positive depending on the local temperature and the concentration of the surface-active elements [10,11]. Oxygen exists generally in atmosphere or shielding gases. The effect of oxygen on Marangoni convection in laser-assisted additive manufacturing has been studied experimentally and numerically [9,12]. For most general-quality forged steel, including low-carbon steel, medium-carbon steel and stainless steel, containing sulfur is inevitable due to the metallurgical imperfection [13]. Addition of sulfur-free powder leads to the redistribution of sulfur in the melt pool. However, the influence of sulfur in the base metal on Marangoni flow during laser-based powder deposition has not been fully understood.

Due to high temperatures, the block of metallic powder and spatter, and small dimension of melt pool, experimental observation is difficult [8]. Numerical simulation has previously offered a tool of effective evaluating the transport phenomena in laser-based powder deposition [14–21]. Qi et al. developed a 3D transition numerical model in which fluid flow is solved with an energy equation [14]. The level-set method was used to capture the free surface of the melt pool. He et al. simulated the laser-assisted additive manufacturing processing by a self-consistent mathematical model [15]. The heat transfer, phase changes, mass

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addition, fluid flow were incorporated in the model. Since the addition of powder results in solute redistribution during the laser-assisted additive manufacturing process, the solute transport in the melt pool has been computed by solving the species conservation equations [16,17]. The solute transport and composition profiles evolution during single-track and double-track laser-assisted additive manufacturing have been reported [16,17]. In these models, the temperature coefficient of surface tension is assumed to be a constant. Lee et al. considered the temperature-varying temperature coefficient of surface tension in stationary Inconel 718 laser cladding [18]. Two opposing surface flows were found within the melt pool. A transition temperature dividing the two regions has been obtained. Although the relationship between surface tension of liquid metal and both temperature and surface-active element content has been established theoretically [22], this surface tension model has not been introduced into the mathematical model of laser-assisted additive manufacturing.

In this paper, in order to investigate the transitional Marangoni convection in laser-based powder deposition on sulfur-containing base metal, an improved surface tension model is proposed to take into account the influence of sulfur content and temperature at the top of melt pool. The sulfur mass transport equation is also combined with the other conservation equations. The Marangoni flows in the melt pool under various mass flow and energy input are examined. The calculated concentrations of elemental sulfur and melt pool geometry are compared with corresponding experimental results to validate the computational solutions.

2. Mathematical model

A numerical model to simulate heat transfer, fluid flow and mass transfer in laser-assisted additive manufacturing has been developed. Fig. 1 shows the physical phenomena in laser-assisted additive manufacturing on the sulfur-containing base metal. The simplifying assumptions are the following [16,21]:

1. The fluid flow in the melt pool is assumed to be Newtonian, laminar and incompressible.
2. The surface tension of liquid metal depends on the temperature and sulfur content at the top of the melt pool.
3. The laser heat flux is assumed to be a Gaussian distribution.
4. The heat flux of the heated powder and the heat loss by evaporation are neglected.
5. The mushy zone where the temperature is between the solidus and liquidus is assumed as a porous medium with isotropic permeability.
6. The concentration distribution of powder flow is assumed to be Gaussian.
7. Powder falling in the region of melt pool is melted immediately. The powder particles are supposed to be at the same temperature as the melt pool and Momentum quantity associated with the powder addition in the melt pool is neglected.
8. There is no diffusion transport in solid phase.

2.1. Governing equations

The following equations of continuity, momentum, energy and solutions transport in the workpiece are expressed in Eqs. (1)–(4).

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\mu \frac{\partial u_j}{\partial x_i}\right) - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_j}{\partial x_i}\right) - K_0 \frac{(1-f_l)^2}{f_l^3 + B} u_i \tag{2}$$

$$\frac{\partial(\rho c_p T)}{\partial t} + \frac{\partial(\rho u_i c_p T)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) - \frac{\partial \Delta H}{\partial t} - \frac{\partial(\rho u_i \Delta H)}{\partial x_i} \tag{3}$$

$$\frac{\partial(\rho c)}{\partial t} + \frac{\partial(\rho u_i c)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial c}{\partial x_i}\right) \tag{4}$$

where t is the time, u_j is the j^{th} component of velocity, μ is the viscosity, p is pressure, and T is the Temperature, c_p is the specific heat, ρ is the density, k is the thermal conductivity, c and D are the concentration and the diffusion factor of the element sulfur. The fourth term in the right side of Eq. (2) represents the frictional dissipation in the mushy zone [23]. K_0 is the morphology constant of the porous media (10^7 in this study). B is a small number to avoid division by zero (10^{-3} in this study). The mass transport of sulfur is calculated based on Eq. (4). ΔH is the latent enthalpy content of the fusion, which is given as,

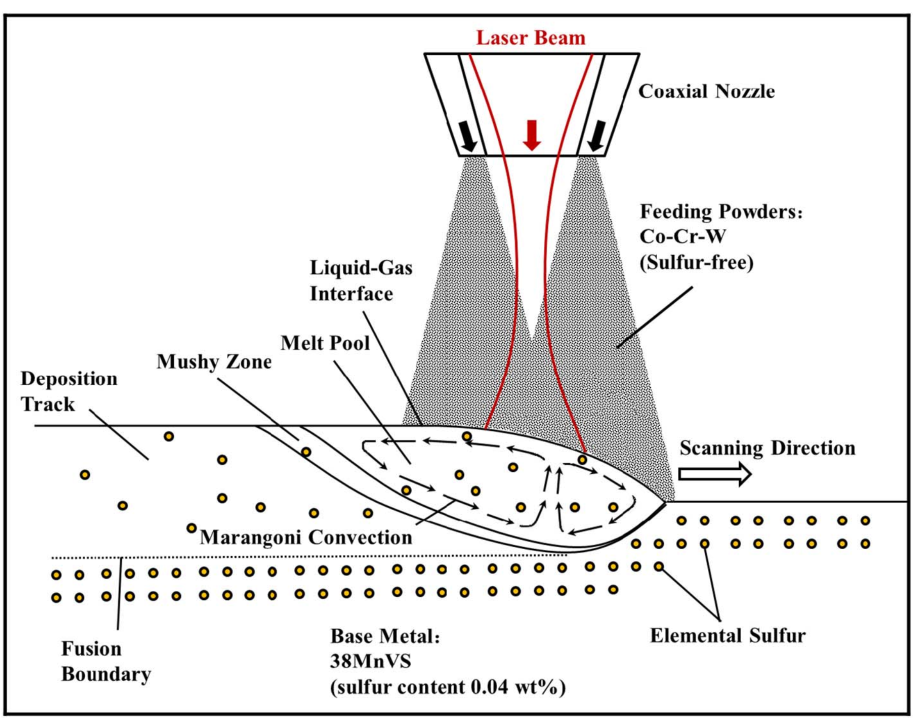

Fig. 1. Modeling Marangoni flow and sulfur mass transport during the laser-assisted additive manufacturing process.