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Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones

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This study demonstrates the significant effect of the recoil pressure and Marangoni convection in laser powder bed fusion (L-PBF) of 316L stainless steel. A three-dimensional high fidelity powder-scale model reveals how the strong dynamical melt flow generates pore defects, material spattering (sparking), and denudation zones. The melt track is divided into three sections: a topological depression, a transition and a tail region, each being the location of specific physical effects. The inclusion of laser ray-tracing energy deposition in the powder-scale model improves over traditional volumetric energy deposition. It enables partial particle melting, which impacts pore defects in the denudation zone. Different pore formation mechanisms are observed at the edge of a scan track, at the melt pool bottom (during collapse of the pool depression), and at the end of the melt track (during laser power ramp down). Remedies to these undesirable pores are discussed. The results are validated against the experiments and the sensitivity to laser absorptivity is discussed.

1. Introduction

Additive manufacturing (AM) is paving the way toward the next industrial revolution [1]. The essence of this advancement is a part that is produced from a digital model by depositing material layer by layer, in other words, 3D printing the model. This technique is in contrast with the traditional subtractive and formative manufacturing approaches. It also eliminates most of the constraints that hinder optimal design, creativity and ease of manufacturing of complex parts [2] [3].

A promising future is in store for L-PBF AM. However, widespread adoption of L-PBF with metallic parts hinges on solving a main challenge: the requirement that the final product should meet engineering quality standards [4]. This includes reducing porosity, since pore defects have one of the most adverse effect on mechanical properties. Experimental advances on this front rely on trial and error methods, which are costly and time inefficient. An attractive alternative to answering this challenge is through modeling and predictive simulation.

The finite element method (FEM) is the most popular numerical method for simulation of metal powder bed additive manufacturing processes. Critical reviews by Schoinochoritis et al. [5] and King et al. [6] discuss different FEM models, assumptions and results. The emphasis is how to get the most out of FEM simulations while avoiding computational expense. Some simplifications include (1) treating the powder as a homogeneous continuum body with effective thermomechanical properties (2) treating the laser heat source as a homogeneous model that deposits laser energy volumetrically like with De-Beer-Lambert's law or one derived for deep powder bed [7], and (3) ignoring melt pool dynamics and therefore assuming a steady state. Take for example the work of Gu et al. [8] who employ a commercial code based on the finite volume method (FVM) to highlight the significant effect of Marangoni convection on heat and mass transfer in a continuum 3D model. In that model, the discrete nature of the powder is not accounted for; hence the melt flow is symmetric along the melt track and does not exhibit fluctuations that may be introduced by a randomly packed

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powder bed.

The current paper falls outside the FEM body of work. Our approach is to study the L-PBF problem with a fine-scale model that treats the powder bed as randomly distributed particles. There are few studies that follow this mesoscopic approach.

In Refs. [9], Gutler et al. employ a volume of fluid method (VOF) and were the first to show more realism with a 3D mesoscopic model of melting and solidification. However, a single size powder arranged uniformly was represented at a coarse resolution that does not resolve the point contacts between the particles. The paper makes qualitative correlations with experiments.

Körner et al. [10] use the lattice Boltzmann method (LBM) under the assumption that the electron beam melting process can be represented in 2D. One big hurdle in this method is the severe numerical instabilities occurring when accounting for the temperature. Körner uses the multi-distribution function approach to reduce these limitations under the assumption that the fluid density is not strongly dependent on temperature. The method has been applied in 2D to study single layer [11] and layer upon layer consolidation [12], and shows the importance that the powder packing has on the melt characteristics. Their observation of the undesirable balling effect was attributed to the local powder arrangement [11]. Recently, a 2D vapor recoil pressure model was added in Ref. [13] to improve the melt depth predictions. The Marangoni effect is neglected. In Refs. [14], a 3D model that does not include recoil, Marangoni, or evaporation effects was used to establish process strategies suitable to reduce build time and cost while enabling high-power electron beam applications.

Khairallah et al. in Ref. [15] reported on a highly resolved model in 3D that considers a powder bed of 316L stainless steel with a size distribution taken from experimental measurements. Khairallah et al. emphasized the importance of resolving the particle point contacts to capture the correct reduced effective thermal conductivity of the powder and the role of surface tension in breaking up the melt track into undesirable ball defects at higher laser scan speeds due to a variant of Plateau-Rayleigh instability theory [16].

A recent mesoscopic study by Lee and Zhang [17] introduces the powder into the model using the discrete element method. Their VOF study emphasizes the importance of particle size distribution and discusses the smoothing effect of small particles on the melt. They agree with Khairallah et al. [15] that balling is a manifestation of Plateau-Rayleigh instability and add that higher packing density can decrease the effect. Recoil and evaporation effects are neglected.

Recently, Qiu et al. [18] performed an experimental parameter study, whereby the surface roughness and area fraction of porosity were measured as a function of laser scan speed. They noted that the unstable melt flow, especially at high laser scan speed, increases porosity and surface defects. Based on a CFD study of regularly packed powder of a single large size of 50 μm, they believe that the Marangoni and recoil forces are among the main driving forces for the instability of melt flow.

This manuscript describes a new high fidelity mesoscopic simulation capability developed to study the physical mechanisms of AM processes by eliminating certain physical assumptions that are prevalent in the literature due to modeling expense. The model uses a laser ray tracing energy source and is in 3D to account for the fluid flow effects due to the recoil pressure, the Marangoni effect, and evaporative and radiative surface cooling. The new findings point out the importance of the recoil pressure physics under the laser and its dominant effect on creating a topological depression (similar to a keyhole) with complex strong hydrodynamic fluid flow coupled to a Marangoni surface flow. A vortex flow results in a cooling effect over the depression, which coupled to evaporative and radiation cooling over an expanded recoiled surface, regulates the peak surface temperatures. This finding should benefit part scale and reduced order modeling efforts, among others, that limit heat transfer to just conduction and therefore suffer from uncontrolled peak surface temperatures and may have to resort to model calibration to capture the effect.

This study, other than detailing the dominant physics in L-PBF, reveals the formation mechanisms for pore defects, spatter, and the so-called denudation zone where powder particles are cleared in the vicinity of the laser track. Several authors report experimentally observing these effects, however, they formulate assumptions for formation mechanisms since, experimentally, it is challenging to dynamically monitor the L-PBF process at the microsecond and micrometer scales. For example, Thijs et al. assume that some particles located in the denudation zone melt incompletely and create pore defects [19] and that other pores form due to the collapse of a keyhole [20]. Qiu et al. [21] observe open pores and assume that the incomplete re-melting of the previous layer generates spherical pores.

The present study explains how three kinds of pore defects (depression collapse, lateral pores, open and trapped pores) are generated and discusses strategies to avoid them. This study, thanks to the laser ray tracing energy source and the inclusion of recoil pressure, is also able to describe the physical mechanisms behind sparking [22], spattering, and denudation [23] [24].

Experimental validation with sensitivity to the choice of laser absorptivity is also presented. The model makes use of the ALE3D [25] massively-parallel multi-physics code. Code details and stainless steel material properties can be found in Ref. [15] [26].

2. Model: underlying physics and validation

2.1. Volumetric versus ray tracing laser heat source

L-PBF is a heat driven process, which needs to be modeled accurately. This study uses a ray tracing laser source (200 Watts) that consists of vertical rays with a Gaussian energy distribution ($D4\sigma = 54$ μm) scanning at 1.5 m/s. The laser energy is deposited at the points of powder-ray intersections. To reduce the computational complexity, the rays are not followed upon reflection. The direct laser deposition is an improvement over volumetric energy deposition (energy as a function of fixed Z-axis reference) used commonly in the literature. Firstly, in reality the heat is generated where the laser rays hit the surface of the powder particles and diffuses inward, whereas homogeneous deposition heats the inner volume of the particle uniformly. Secondly, the rays track the surface and can reproduce shadowing. In Fig. 1a, a 150W Gaussian laser beam is initially centered above a 27 μm particle sitting on a substrate and moved to the right at 1 m/s. For volumetric energy deposition, melting happens simultaneously everywhere inside the particle. The wetting contact with the substrate increases rapidly, which artificially increases heat dissipation. On the other hand, with realistic laser ray tracing, melting is non-uniform as it occurs first at the powder particle surface. More heat accumulates inside the powder particles compared with the homogeneous laser deposition because it releases to the substrate slowly through a narrow point contact. If insufficient heat is deposited, the particles are partially melted and contribute to surface and pore defects as discussed in section 3.2.5. The laser ray tracing heat source helps to better couple the physics behind surface heat delivery and melt hydrodynamics.

2.2. Temperature driven 3D flow effects: surface tension, Marangoni convection, and recoil pressure

Fig. 1b, c and d illustrate the significant change of melt pool