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Prediction of microstructure in laser powder bed fusion process

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ABSTRACT

Additive manufacturing (AM) processes are receiving widespread attention due to the ability to create or repair precision engineering components without use of any die or mold. Currently, the approach to obtain a specific user defined/as-desired or conformal/epitaxial microstructure is a challenging and expensive iterative process. Modeling and validation of solidification microstructure can be leveraged to reduce iteration cost in obtaining a desired microstructure. Numerical Volume-of-fluid based method incorporating Marangoni convection can accurately predict the resultant melt pool geometry and temperature distribution which can serve as an input in prediction of microstructure evolution in solidifying mushy region. Hence, in the present study, computational fluid dynamics (CFD) analysis is used to predict melt pool characteristics and phase field modeling is employed to simulate microstructure evolution in the as-deposited state for laser powder bed fusion (LPBF) process. Different features of LPBF microstructure such as segregation of secondary elements, dendrite sizes, dendritic orientation, dendritic morphology, and surface roughness are investigated and validated through comparison with experimental results. Phase-field model suggests strong dependency of dendrite orientation on surface roughness and scan speed and suggests potential of columnar flip or oriented-to-misoriented transition at higher scan speed. Segregation of the secondary elements is found to be the dominant factor in resultant dendrite width in the range of 1–3 μm. Furthermore, the developed method can easily be extended to predict the change in orientation of dendrites as new layers are built atop previous layers.

1. Introduction

Additive manufacturing (AM) methodologies, such as laser powder bed fusion (LPBF), selective laser melting (SLM), laser beam melting (LBM) and electron beam melting (EBM), enable the fabrication of complex metal, alloy, polymer, ceramic, and composite structures by the freeform construction of the material, layer by layer. These additive manufacturing techniques allow for the fabrication of fully-dense metallic components directly from three-dimensional geometry solid models developed in computer aided design (CAD) software systems. The parts can have complex topology and even contain intricate internal structures, such as vascular or with special porous shapes or lattices, cooling paths, etc. [1–5].

The overall concept of AM systems involves the selective melting of a powder or wire feedstock by a directed energy source (laser or electron beam), producing the layer-by-layer buildup of material. Feedstock melting occurs in a localized region of the energy beam, producing small volumes of melting, called melt pools, followed by rapid solidification, allowing for very precise control of the solidification process during fabrication. The end result is the ability to manufacture precision near net-shape engineering components in one step for varied engineering requirements.

LPBF starts by spreading a bed of alloy feedstock powder. A laser selectively melts and fuses powder particles together. After each solidification cycle, the build plate moves down for a layer thickness and the next layer of alloy powder is deposited on top of the already manufactured part. An important aspect of the LBPF is the rapid heating of the feedstock by the traversing energy beam melting the powder, followed by rapid cooling, and re-solidification. This process produces high temperature gradients that induce circulation of the molten material driven by surface tension gradients and non-equilibrium of the solid/liquid interface, including incomplete melting/sintering. Re-solidification results in shrinkage of the powder to typically half of its volume and gas entrapment are known to play a large role in the orientation of the grain growth, porosity, residual stresses, and defects in the microstructure. The grain structure is affected by the temperature

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gradients, as well as by the previously solidified layer's grain structure.

In order to help designers to employ AM technology, quality and lifing of AM components must be understood, especially for metallic parts with defects, hence certification of the final component needs to match the strength requirement. Monitoring part quality is paramount to avoid buildup of residual stress, cracks, porosity and to reduce detrimental segregated phases commonly observed during alloy solidification. Simulation plays a huge role in predicting the melt pool dimension and can be used to optimize the process parameter [6]. There is a current industry need to exploit the benefits of AM technology by improving the mechanical properties of end-use production parts, faster design-to-product times. It cannot be achieved without understanding of the effects of input AM process parameters, microstructure, defects and grain orientation. Prediction of the as-deposited microstructure is important in two regards. First, AM technology has the advantage of fabricating parts near net shape. While this reduces the required number of machining steps, components often require a series of expensive and timely post build operations to include stress relief, hot isostatic pressing as well as any homogenization and strengthening heat treatments (solution and age hardening). Understanding as-deposited grain morphology and chemical segregation will reduce the number of iterations required to hone in on optimal post processing heat treatments. Second, predicting the as-deposited structure will bolster part consistency. Confidence that a set of process parameters will provide the same as-deposited structure will aid in part qualification. DeHoff et al. [7] has shown how AM process parameters can influence the thermal gradient and solidification velocity resulting in variations in grain orientation from equi-axed to columnar to a mixture of both.

The solidification rates in AM are fast (cooling occurs at 10^5–10^6 °C/s [6]) and the nonequilibrium kinetics need to be incorporated in the partitioning factor to simulate the rapid solidification. Rapid solidification of the multiple layers of small melt pools generates specific microstructure that might be detrimental for the part performance in service conditions. An optical image of an etched cross section for a bulk LPBF coupon of IN718 in Fig. 1 reveals the scallop like structure from the melt pools solidified during each layer of the build. From the contrast, it is possible to identify clusters of dendrites that span multiple layers/melt pools. This feature likely stems from partial re-melting of the previous layer with the dendrites seeding off of this prior layer during solidification. Inconel 718 (IN718) is used as disc and turbine blade alloy in high compressor, burner and turbine modules of contemporary turbine engines. IN718 is used in complex wrought, welded assemblies such as the diffuser cases and TOBI (tangential on board injection) [8]. Homogenization heat treatments have been developed to minimize the impact of the as-cast segregation, and hot isostatic pressure technology (HIP) is used to reduce both the presence of as-cast porosity and segregation, further improving the quality of cast IN718 components. Nevertheless, wrought IN718 parts exhibit superior properties over the cast parts. Traditional production of casting and especially wrought superalloys requires laborious procedures [9]. Thus, the goal to achieve the properties of wrought IN718 using AM techniques is extremely important and attractive. Solidification is a non-linear phase transformation process that leads to the formation of complex microstructures. Depending on the particular characteristics of the material processing the final microstructure might vary significantly. The most common metal and alloys microstructure that formed during undercooled solidification has a dendritic pattern. These complex dendrite microstructures have significant effects on the mechanical and material properties of cast alloys. The multi-scale nature and complexity of solidification patterns, however, make the understanding and prediction of these patterns extremely difficult [10]. Different mathematical approaches have been developed to study the dendritic growth during solidification, falling basically into two categories, sharp interface and phase field methods. The classical mathematical formulation is so-called Stefan problem with a free moving boundary. This is the sharp-interface model approach [11–13] consisting of two sets of thermal-diffusion equations in the liquid and solid regions, coupled by boundary conditions defined at the solid-liquid interface. The local velocity of the interface and its position is calculated during the problem solution and accounted for the interfacial mobility, curvature, and heat flux at the interface. It is numerically challenging problem especially for the case of geometrically complex multiple interfaces (multi-connected regions specific for multiple dendritic growth). For this reason a considerable effort has been put into developing alternative numerical approaches, particularly, phase-field methods allowing simulation without explicit treatment of free boundaries. The diffused interface approach recognizes that real interfaces have finite thickness where physical quantities vary from their bulk values [14]. In the binary phase field method, the state of the entire microstructure is represented continuously by a single variable known as the order parameter, $0 < \varphi < 1$. Bulk phases are represented by constant values of phase indicator, for example in the liquid and in the solid, while the interface corresponds to the domain where phase indicator changes. Thus, the energy term describing interface is a function of $\nabla\varphi$, because only in this region the order parameter varies between the values specified for both phases. The total free energy is then described in terms of the order parameter, φ, and its gradients. Phase field (or diffuse) methods are based on minimization of the system free energy including gradients of the thermodynamic variables accounting for non-local effects.

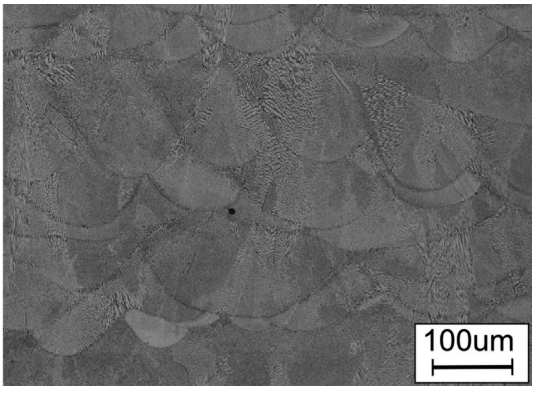

Fig. 1. Optical image of bulk coupon cross section highlighting the melt pools at each build layer for IN718.

All state variables and parameters in this approach depend on the phase indicator, and subsequently, automatically change with the evolution of the structure. Thus, with a single energy functional to describe the evolution of the phase field, coupled with constitutive equations for each phase, one can describe the process irrespective of the number of phase domains in the system. It is important to note that the locations of the interfaces no longer need to be tracked, but can be calculated from the evolution of field parameters.

During the solidification the microstructural evolution occurs to reduce the free energy of the system and force the system to a low energy equilibrium condition. The solidification calculations typically performed at a mesoscopic space scale of typically 1 μm [15]. Coupled thermal-phase and field-concentration equations can be