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Simulation and analysis of γ-Ni cellular growth during laser powder deposition of Ni-based superalloys

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ABSTRACT

Cellular or dendritic microstructures that result as a function of additive manufacturing solidification conditions in a Ni-based melt pool are simulated in the present work using three-dimensional phase-field simulations. A macroscopic thermal model is used to obtain the temperature gradient G and the solidification velocity V which are provided as inputs to the phase-field model. We extract the cell spacings, cell core compositions, and cell tip as well as mushy zone temperatures from the simulated microstructures as a function of V. Cell spacings are compared with different scaling laws that correlate to the solidification conditions and approximated by $G^{-m}V^{-n}$. Cell core compositions are compared with the analytical solutions of a dendrite growth theory and found to be in good agreement. Through analysis of the mushy zone, we extract a characteristic bridging plane, where the primary γ phase coalesces across the intercellular liquid channels at a γ fraction between 0.6 and 0.7. The temperature and the γ fraction in this plane are found to decrease with increasing V. The simulated microstructural features are significant as they can be used as inputs for the simulation of subsequent heat treatment processes.

1. Introduction

Ni-based superalloys possess excellent mechanical properties at elevated temperatures, which make them suitable for gas-turbine and jet-engine components [1]. The laser powder bed fusion (L-PBF) additive manufacturing (AM) process is used to produce near net-shaped metallic parts from the alloy powder, in a layer-by-layer fashion with multi-pass laser melting, solidification and solid-state phase transformations, in a shorter manufacturing time than traditional casting, metal forming, and machining processes, with almost no waste and at a reasonable cost [2,3]. Solidification in this process controls the size, shape and distribution of the γ grains, the growth morphology, the elemental segregation and precipitation, the solid-state transformations and ultimately the properties and performance of the product. Understanding and predicting the melt pool solidification behavior is therefore important.

Additive manufacturing is a relatively new research field. Some of the outstanding issues in this process are related to the cell/dendrite spacing, microsegregation and residual stress [3] in the as-deposited parts. Several experimental investigations [2,4–8] and numerical simulations [9–13] have linked the AM process parameters to the melt pool solidification conditions – temperature gradient G and solidification velocity V – on a microscopic scale. The growth morphologies that result as a function of the solidification conditions and intercellular segregation determine the yield strength, ultimate tensile strength and fatigue strength of the material [14]. The solidification conditions considered in previous studies have been relatively small-valued. For example the cooling rates, $\dot{T} = GV$, were reported to be no higher than $10^4\ \mathrm{K\,s^{-1}}$, whereas the present work treats larger values ($\dot{T} = 10^6\ \mathrm{K\,s^{-1}}$) of the melt pool solidification conditions. Therefore, the characteristic cell spacings, concentrations and temperatures in the parameter-microstructure map are expected to be different from those reported in the existing literature.

Cell spacing depends on melt pool solidification conditions G and V [7,14,15] and is often estimated as $\lambda_c = AG^{-m}V^{-n}$, where m and n are the model-dependent exponents and the coefficient A depends on alloy properties. During solidification, solute is partitioned between the solid and liquid phases, and in ideal conditions reaches the corresponding equilibrium values of the phase diagram. Such solute partitioning however is incomplete in the AM solidification regime and therefore the solute concentration field predicted by the phase diagram no longer applies [10,16]. In order to reflect this departure from equilibrium, solidification parameters in the theories are phenomenologically modified from equilibrium to velocity-dependent values [10,17]. The above theories are

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used as a reference to compare with our spacing and microsegregation simulation data.

The mushy zone in cellular microstructures is a two-phase solid and liquid coexistence region between the fully solid and the fully liquid states where the majority of the solidification defects form [18,19]. These defects arise due to the random growth of the solid cells towards one another which finally coalesce and thereby restrict the feeding of the liquid to accommodate shrinkage during late solidification stages. As the solid fraction in the mushy zone increases, the liquid is not able to flow freely and compensate for shrinkage, resulting in microporosity. The semisolid mushy zone therefore becomes weak and ruptures when stressed in a phenomenon called hot tearing. Although we have not considered fluid flow in the present model, mushy zone solidification behavior is estimated by the solid and residual liquid fractions during coalescence of the γ cells.

Diffusion of solute is significantly different in 3D than that in 2D, which results in different velocities, compositions and temperatures of the growing cells/dendrites [9,12]. Lee et al. [9,12] have studied the dendrite growth problem in 2D and 3D with and without convection. Their simulations suggest that dendrites are finer in 3D and grow twice as fast in comparison to 2D. Interestingly, the difference in solute mass fraction at the 3D dendrite core with and without convection was less than 0.01% and the dendrite tip properties such as shape and curvature remained similar in both cases. The topological features of the solid and liquid phase interaction are far more complex in 3D than that in 2D, which makes analysis of the mushy zone difficult. The present work catalogs the above differences that arise from both 2D and 3D simulations in AM solidification conditions.

Solidification in the melt pool begins at the fusion boundary, and G and V are found to vary along this boundary. As in [20], G and V values are estimated from a 3D heat transfer finite element simulation for use in a phase-field model for microstructure simulation. The phase-field solidification model is described in Section 2. Cellular solidification microstructures are presented and analyzed in Section 3. The general results are discussed in Section 4 and conclusions are drawn in Section 5.

2. Phase-field solidification model

The phase-field method is one of the most powerful computational techniques to simulate three-dimensional dendritic growth in binary alloys [21,22]. We have used a phase-field model that has been detailed in Refs. [23,24]. This model quantitatively simulates the time-dependent evolution of a non-conserved phase-field ϕ and the conserved composition field c during solidification of a dilute binary alloy. The phase-field ϕ is a scalar-valued order parameter field which distinguishes the microstructure phases; $\phi = 1$ in the solid, $\phi = -1$ in the liquid and the solid-liquid interface is described by $-1 < \phi < 1$. This approach avoids explicit tracking of the interface and thus the complex solid-liquid surfaces are extracted in an efficient way [25–28]. An anti-trapping solute flux term was introduced in this model to avoid unphysical solute-trapping effects due to the use of large numerical interface thickness values at low solidification velocities. However, we will show below that the model does not prevent solute-trapping at AM solidification velocities. The effects of melt convection are not included in this model and thus solute is transported in the liquid by diffusion only. The evolution equation for ϕ in 3D is expressed as

$$\tau_0 a(\hat{n})^2 \frac{\partial \phi}{\partial t} = W_0^2 \nabla \cdot \left[a(\hat{n})^2 \nabla\phi\right] + \sum_{i=1}^{3} \partial_i \left[a(\hat{n}) \frac{\partial a(\hat{n})}{\partial(\partial_i \phi)} |\nabla\phi|^2\right] + \phi - \phi^3 - \frac{\lambda}{1-k_e}(1-\phi^2)^2 \left[\exp(u) - 1 + \frac{G(z-Vt)}{m_l c_0/k_e}\right]. \qquad (1)$$

The dimensionless surface energy function $a(\hat{n}) = 1 - \epsilon\left[3 - 4(n_x^4 + n_y^4 + n_z^4)\right]$ represents the three-dimensional four-fold anisotropy at the solid–liquid interface with strength ϵ and n_i is the interface normal vector pointing into liquid along the Cartesian direction, i, in the lab frame of reference. Alloy composition c_0, liquidus slope m_l, and equilibrium partition coefficient k_e are taken from a Ni-Nb phase diagram [29]. $k_e = c_s/c_l$, where c_s and c_l are the equilibrium compositions on the solid and liquid side of the interface. The dimensionless chemical potential u is given by $\ln\left(\frac{2ck_e/c_0}{1+k_e-(1-k_e)\phi}\right)$. A frozen-temperature approximation is applied in which the temperature gradient G is translated along the z (growth) axis with a velocity V.

The evolution equation for c is given by

$$\frac{\partial c}{\partial t} = -\nabla \cdot \left[-\frac{1}{2}(1+\phi) D_l c \exp(u)^{-1} \nabla \exp(u) + \frac{1}{2\sqrt{2}} W_0 (1-k_e) \exp(u) \frac{\partial\phi}{\partial t} \frac{\nabla\phi}{|\nabla\phi|}\right], \qquad (2)$$

where the first term inside the square bracket represents a standard Fickian diffusion flux and the second term is the anti-trapping solute flux. D_l is the diffusivity of solute in the liquid.

The numerical parameters in this model, W_0: the interface thickness, τ_0: the phase-field relaxation time, and λ: a dimensionless coupling constant, are linked to the material properties via the chemical capillary length $d_0 = a_1 W_0/\lambda$ and the time scale for diffusion $\tau_0 = a_2 \lambda W_0^2/D_l$ using a thin-interface analysis which makes the interface kinetics vanish. The numerical constants are given by $a_1 = 0.8839$ and $a_2 = 0.6267$, after Ref. [23]. Both W_0 and τ_0 values are used to render all the simulation parameters dimensionless.

2.1. Simulation setup

In order to study microstructure evolution, ϕ (Eq. (1)) and c (Eq. (2)) equations of motion are solved on a uniform mesh, using a finite volume method and an explicit time marching scheme. A zero-flux boundary condition is applied on both ϕ and c fields in all directions. The size of the simulation box in the growth (z) direction is taken as 10 μm, which is at least 50 times the diffusion length D_l/V, and varying domain sizes, $L_x \times L_y$, are used ranging from 2 μm × 2 μm to 4 μm × 4 μm depending on the fineness of the γ cells simulated. For each simulation, a grid spacing $\Delta x/W_0 = \Delta y/W_0 = \Delta z/W_0 = 0.8$ and a time step $\Delta t/\tau_0 = 0.05$ are used. An interface width of $W_0 = 0.01$ μm, corresponding to $\lambda = 1.38$, is used.

Each simulation begins from the bottom of the simulation box with a thin solid layer of height 0.05 μm and with an initial Nb composition of $k_e c_0$ in the solid and c_0 in the liquid. Small, random amplitude perturbations are applied at the initial solid-liquid interface, from which stable perturbations grow with time and break into steady state γ cells. After these cells have grown to a pre-defined length, we translate the box upward and in doing so the solid in the bottom of the box is removed. This approach does not modify the dynamics of the cellular solidification front since there is negligible diffusion in the solid, but saves a considerable amount of computation time and storage.

2.2. Parameter details

It should be noted that we have approximated the Inconel 718 (IN718) multicomponent alloy to be a binary Ni-5%[1] Nb in this

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[1] Concentration is represented in mass fraction in the present paper.