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Modeling of binary alloy solidification under conditions representative of Additive Manufacturing

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ABSTRACT

Understanding the interplay among process parameters, microstructure, and presence of defects is critical to optimizing Additive Manufacturing (AM) routes for producing specialty alloy parts with unique geometry, properties, and compositional features. However, since it is not feasible to obtain experimental results for every possible set of AM process, process conditions, and alloy composition, computational modeling is becoming an increasingly important tool for understanding key physical processes, with the hope of developing a framework for AM materials design. One such physical process of interest is the dendritic solidification within grains; we implement a Cellular Automata (CA) model for coupled solute transport and growth of cellular and dendritic β-Ti alloy colonies under thermal conditions typically encountered in AM processes. Quantitative agreement with analytical models of the undercooling-solidification velocity relationship was achieved, as well as qualitative agreement with trends in primary dendrite arm spacing (PDAS), secondary arm development, and compositional profile with changes in solidification conditions. The roles of solute diffusivity, interfacial energy, and alloying addition are considered as well. Under rapid solidification conditions, extension to include local non-equilibrium for solute allowed for the modeling of solute trapping along dendrite stems as well as qualitative representation of the dendritic to banded morphology transition. To quantitatively reproduce non-equilibrium solidification at the dendritic colony scale and more accurately estimate rapid solidification microstructures, use of multiple grids or more complex CA rules would be in order.

1. Introduction

The development of solidification conditions during additive manufacturing (AM) is a complex and multiscale process, depending strongly on the details of the specific AM method used (e.g., laser vs electron beam based, or powder-bed vs. direct deposition) [1]. As the material absorbs energy, features of the molten pool (size, shape, temperature profile, etc.) will vary based on the various potential modes of heat transport in the system. In particular, advective heat transport arising from strong surface-tension driven fluid flow [2–4] may significantly alter the molten pool. Many other factors have a significant affect on the molten pool size as well [5], including the enthalpy of mixing for deposition of elemental powder blends [6,7], release and absorption of latent heat due to the solid-liquid phase transformation, and motion of the energy source [8–10]. Local cooling rates and thermal gradients vary strongly as functions of position and time owing to these melt pool dynamics. The temperature field in the wake of the energy source along with the thermodynamics and kinetics of the solidification process in turn play a significant role in the development of microstructure and porosity [10,11]. Differently-orientated grains along the constrained solidification front will impinge as they grow in the direction of the local thermal gradient, often leading to the dominance of a preferred orientation [12]. This growth typically results in a heavily textured, columnar grain structure [13–16]. However, by tuning process parameters such as scan pattern and altering the composition of the materials used, it has been shown that tailoring of texture, grain size, grain morphology, and phase is possible for various alloys [10,17–21]. Experimental results show that these grain structures and microstructural features are directly related to mechanical properties in AM parts [13,22], making them, and the conditions that lead to their development, important for optimizing AM processes.

While the highly localized nature of the process and myriad process variables that effect physical phenomena in and around the molten pool lead to challenges for process optimization, there is also significant opportunity from a materials design perspective. AM deposition processes offer the unique ability to control the solidification conditions by altering process parameters such as material composition and input energy density. Understanding and controlling the factors that play

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roles in the development of features such as texture, residual stress, and grain size enables the use of AM to build parts with locally tailored properties. In a previous work [23], we presented results from modeling dendritic colony growth as a function of fluid and heat transport conditions representative of Laser Engineered Net Shaping (LENS™) – a direct deposition based AM process. That work was performed using a lattice Boltzmann-cellular automaton (LB-CA) method for coupled modeling of fluid flow, solute transport, and solidification. Here, we further investigate the qualitative and quantitative effectiveness of this model for constrained solidification of multiple binary β-Ti alloy systems for the solidification conditions expected in the LENS™ process. The focus of the present work is on the role of solidification conditions on the as-solidified columnar intra-grain microstructure in β-Ti binary alloy systems; as previously mentioned, multiple grains with various orientations will be present and impinge as thermal conditions vary across the melt pool under real AM conditions. We focus on the trends in the morphology inside an individual grain (with fixed orientation) in order to understand microstructure development as a first, but necessary, step towards designing an alloy and the specific set of process conditions for AM deposition.

2. Background

Binary alloy solidification has been modeled extensively in the literature with various methods and for various conditions. For the purposes of this work, solidification of a single solid phase under the constrained solidification conditions described by Trivedi and Kurz is considered [24]. These conditions are common at the edge of the molten pool in beam-based processes, with assumptions of a positive thermal gradient ahead of a locally planar solid-liquid interface, no nucleation of solid in the bulk liquid ahead of the interface, and latent heat released on solidification conducted through the solid with no effect on the thermal gradient in the liquid. When the local temperature places the material between the solidus and liquidus curves, solidification will begin at a composition different from that of the overall alloy. Partitioning of solute between the two phases and diffusion-limited solute transport in the liquid will give rise to a gradient in solute concentration ahead of the interface. If the magnitude of the solidification velocity V exceeds

$$V = \frac{GD}{\Delta T_0} \tag{1}$$

then a region of liquid undercooled relative to the local composition's liquidus temperatures will exist [25]. In Eq. (1), G is the thermal gradient ahead of the solidification front, D is the solute diffusivity in the liquid (assumed here to be independent of temperature), and ΔT_0 is the equilibrium freezing range for an alloy of overall solute concentration C_0. This effect is schematically illustrated in Fig. 1 for the case of a generic alloy system with linear liquidus slope m_L and constant solute partition coefficient k. We present results for two alloy systems, Ti-Cu, which has a phase diagram such as shown in Fig. 1, and Ti-W, which has a liquidus slope that is positive rather than negative, resulting in the solute being more soluble in the solid than the liquid. However, regardless of the sign of the liquidus slope, the following discussion holds.

Under the steady-state operating conditions for LENS™, thermal gradients on the order of 10^5 K/m and cooling rates in the range of 10^3–10^4 K/s are typical [26,27]. The solidification velocities under these conditions easily those characteristic of Eq. (1) and would be expected to lead to the development of an undercooled region ahead of an initially planar solidification front. The mechanisms for the breakdown of this planar interface into cells and the further breakdown of cells into dendrites are dependent on solute diffusion and interfacial energy, and are described extensively in the literature [25,28–31]. This relationship among dendrite tip undercooling, radius, and velocity at steady state is explored in the model of Kurz, Giovanola, and Trivedi (often referred to as the KGT model) as a function of the phase diagram, temperature-dependent solute diffusivity, interfacial energy, and thermal gradient [32]. Assuming a given geometry for the growing cells also allows for analytical modeling of the primary dendrite arm spacing (PDAS) [33], though the accuracy of such models is often limited [24]. While the transition from growing parabolic cells (as described by the Ivantsov dendrite [24]) to truly dendritic structures with secondary and sometimes ternary arms has been modeled by Kurz and Fischer and seen experimentally [24,33], there is no sharp transition with varied cooling rate $\dot{T}$ and thermal gradient G from columnar cellular to dendritic structures but rather a range of solidification rates in which secondary arm development occurs [29]. Beyond this range, the fine PDAS in rapid directional solidification limits the development of secondary arms. With reduced G ahead of the solidification front, the resulting increase in spatial extent of the zone of undercooled liquid gives rise to significant probability of nucleation of new grains that may block the advance of the columnar front [25]. While such a transition between columnar dendritic to nucleated, more equiaxed dendritic grains may occur in the LENS™ process, as modeled in the solidification maps of Bontha et al. for fast solidification rate and low thermal gradient [10,21], the present work focuses on modeling of the columnar dendritic structures and planar interface breakdown. However, it should be kept in mind that at low laser power and fast beam velocities, the solidification regime particularly near the top of the melt pool may transition from one dominated by columnar dendritic grains to one with significant fractions of nucleated grains.

As the solidification rate is increased, the magnitude of the dendrite tip undercooling relative to the liquidus temperature for C_0 increases [25]. A limit of absolute stability, in which the cellular or dendritic front gives way to a stable planar front at the solidus temperature for C_0, occurs at the critical solidification rate [24,25]

$$V = \frac{\Delta T_0 D}{k\Gamma} \tag{2}$$

in which Γ is the Gibbs-Thomson coefficient. Beyond this critical solidification rate, growth is no longer limited by solute diffusion but rather by interface attachment kinetics for atoms joining the solid, a solidification regime not modeled in the present work [24]. However, as the velocity in Eq. (2) is often in the near-rapid or rapid solidification regime, deviation from local equilibrium for solute at the interface and in the liquid must be accounted for. This is due to the fact that the speed at which the dendrite tip is growing is of a similar order of magnitude as the speed at which solute atoms around the tip are diffusing. As a result, there is a solidification velocity-dependence of solute concentrations on both sides of the interface (altering ΔT_0 and k from their equilibrium values), and in turn altering the velocity of Eq. (2). The aforementioned KGT model takes into account the deviation of quantities k, D, and liquidus slope m_L as functions of velocity [32]. The KGT model also takes into account variation in these quantities as a function of temperature, though this was neglected in the present work as the alloy systems modeled had relatively small solidification ranges and therefore minimal variation of these quantities with temperature. Formation of solid with a composition different than that described by the equilibrium phase diagram at a given dendrite tip temperature is referred to as solute trapping, and can occur provided that the process of solidification still lowers the overall Gibbs free energy of the system [24]. Equations for the liquidus slope and solute partition coefficient as functions of V under rapid solidification as modeled by Sobolev [34] are, respectively,

$$k(V) = \frac{k^{eq}\left(1-\frac{V^2}{V_D^2}\right) + \frac{V}{V_{DI}}}{1-\frac{V^2}{V_D^2} + \frac{V}{V_{DI}}},\ V < V_D;\quad k(V) = 1,\ V \geq V_D \tag{3}$$

and