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A sensitivity analysis of the columnar-to-equiaxed transition for Ni-based superalloys in electron beam additive manufacturing

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ABSTRACT

Solidification conditions experienced during Selective-Electron Beam Melting (S-EBM) of Nickel-Base superalloys generally lead to epitaxial grain growth from previous layers, resulting in highly textured columnar grain structures, and consequently, highly anisotropic mechanical properties. However, in recent work, researchers have been able to produce equiaxed grain structures by changing the scan strategy to influence the solidification conditions, thereby obtaining isotropic properties. The competition between columnar and equiaxed grain formation is governed by both the local thermal conditions and alloy thermodynamics. The above examples demonstrate successful manipulation of the thermal conditions through changes in process parameters. However, there is no guarantee that process conditions that encourage the formation of equiaxed grains for a given alloy will coincide with the production of defect free material. The goal of this work is therefore to understand the influence of alloy composition on the columnar-to-equiaxed transition (CET) so that alloys may be designed such that grain structure control is accessible to a wider range of S-EBM process conditions. A CET model originally developed by Hunt and extended by Gäumann was used to relate processing conditions to resulting microstructure. A sensitivity analysis of the CET model was performed using the Element Effects Methods. The results lead to a comparison of the relative effects of various alloying additions on the CET, as well as an assessment of other model parameters, including, most significantly, the nucleation density of equiaxed grains.

1. Introduction

The mechanical properties of Nickel-base superalloys are directly linked to their microstructure, which in turn, are dependent on both alloy chemistry and processing conditions. Existing superalloy compositions were designed with a given process in mind (e.g. investment casting) to engineer a specific microstructure [1,2]. Research in additive manufacturing (AM), with a focus on selective-electron beam melting (S-EBM), has sought to adopt existing alloy compositions (e.g. IN718, IN625, MAR-M247) to these new technologies with a goal of exploiting new design freedoms. Due to high thermal gradients, the grain structure of Ni-base alloys produced using S-EBM generally favor epitaxial growth from previously deposited layers, resulting in highly textured columnar grain structures and associated anisotropic properties [3]. However, it has been shown experimentally [4,5] and through modelling [6,7] that equiaxed grain structures with isotropic properties may be produced using S-EBM through manipulation of process parameters. Consequently, S-EBM produced components could have grain structures that are favorable for the complex loading conditions of a given application.

The competition of columnar grain growth and equiaxed grain nucleation has been studied in the context of both casting [8] and welding [9,10] based on interface response function theory [11], which showed that grain structure development is a function of both the local thermal conditions and alloy thermodynamics. Site-specific grain structure control in S-EBM has focused on manipulating thermal conditions through process parameter selection and scan-strategy design to encourage solidification conditions favorable for equiaxed grain nucleation. These works use IN718, a well-established alloy that is useful for developing an understanding of individual processing parameters. However, as a result, they do not investigate the role of alloy chemistry on microstructure development. Consequently, it is only a coincidence

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that the process window that favors equiaxed grain nucleation in IN718 is wide enough that defect-free material may be produced while simultaneously manipulating the microstructure. Furthermore, this level of understanding limits alloy selection to a trial-and-error approach among pre-existing compositions that were developed for conventional processing conditions. The purpose of this work is therefore to understand the influence of alloy chemistry and other material parameters on equiaxed grain formation, thereby enabling alloy design specifically for microstructure selection in S-EBM.

To understand the influence of alloying elements and other process variables on grain structure development, methodology from the uncertainty quantification (UQ) community has been adopted. UQ methods have been used in solidification modeling [12,13] and demonstrated in additive manufacturing [14] to obtain an understanding of how different model inputs affect an output of interest. UQ allows for establishment of which physical parameters and process controls have the greatest effect on a given outcome and may be used to identify where researchers should focus their efforts to reduce the uncertainty of model predictions. In the present study, the elementary effects technique will be applied to a model for the columnar to equiaxed transition in Ni-base superalloys to quantify the sensitivity of the grain structure development to two distinct sets of inputs. The first set of inputs is the range of alloy compositions that is common within Ni-based superalloys. These inputs are not uncertainties, but rather, are the design space available for tuning the solidification behavior of the resulting alloy. Understanding the influence of different alloying elements will enable researchers to prioritize the selection of elemental compositions to have the greatest impact on solidification characteristics. The second set of inputs is the physical and thermodynamic parameters of the alloy within the selected composition space. These inputs may be classified as epistemic uncertainties [12] in that, theoretically, given a particular composition and set of processing conditions, they may be better characterized, but in the present scenario have a significant level of uncertainty. Thus, this work seeks to understand the viability of Ni-based superalloy design for grain structure control in additive manufacturing, for a given design space, in the context of uncertainties in the alloy properties and physical processing conditions.

2. Methods

The model under consideration is a phenomenological approach to predicting the competition between columnar grain growth and equiaxed grain nucleation. The model itself is presented in Section 2.1. The model is interrogated according to the elementary effects method for determining the sensitivity of the model outputs to each input as described in Section 2.2. Section 2.3 describes the selection process for each input parameter, and Section 2.4 explains the outputs that will be used to quantify the model.

2.1. Calculation of the Columnar-to-Equiaxed transition

The basis of the columnar-to-equiaxed (CET) transition model used here was initially developed by Hunt [8] for casting processes to predict the competition between columnar grain growth and equiaxed grain nucleation. This model assumes that all equiaxed grains ahead of the columnar front nucleate once the local undercooling has reached a critical value, and if they are able to grow above some critical volume fraction, they impede the growing columnar front. The result of Hunt's model is a prediction of the stable grain structure as a function of alloy properties and solidification conditions, specifically the thermal gradient (G) and solid-liquid interface velocity (V_s). Gäumann et al. [9] extended Hunt's model to include high solidification rate effects relevant to laser welding through the incorporation of the Kurz-Giovanola-Trivedi (KGT) model for dendrite growth [15]. For additive manufacturing, solidification rates are high enough for curvature effects at the dendrite tip to become import. Therefore, the present model is adapted from the work of Gäumann et al.

The thermal gradient at which a particular volume fraction of equiaxed grains is formed may be expressed as

$$G = \frac{1}{n+1}\sqrt[3]{\frac{-4\pi N_0}{3\ln(1-\phi)}}\Delta T\left(1-\frac{\Delta T_n^{n+1}}{\Delta T^{n+1}}\right), \tag{1}$$

where N_0 is the nucleation volume density, ϕ the volume fraction of equiaxed grains, ΔT the dendrite tip undercooling for columnar grain growth, n is a material dependent parameter, and ΔT_n the undercooling required for equiaxed grain nucleation. The dendrite tip undercooling consists of four parts: constitutional, curvature, kinetic and thermal undercooling. Under Gäumann's model the curvature, kinetic and thermal undercooling were ignored because their contributions were considered insignificant, while the constitutional undercooling was modeled with the relationship $\Delta T_c = (aV_s)^{\frac{1}{n}}$ to simplify calculations. Under Gäumann's assumptions, a and n served as fitting parameters based on the KGT model for undercooling and the same relationship was used for both columnar and equiaxed dendrite growth. These assumptions are limiting, however because they neglect the influence of the thermal gradient on undercooling, as well as the influence of the dendrite tip curvature, which becomes non-negligible at high solidification velocities such as those found in electron beam additive manufacturing. In this paper, the undercooling was instead directly calculated from the KGT model, removing the need to fit the material parameter a and allowing for a direct relationship between composition and undercooling. This approach also has the effect of separating the growth laws for columnar and equiaxed dendrites, where the former is now dictated by the KGT model, and the latter controlled by the fitting parameter n. The effects of such assumptions are discussed further in section 4.4. Under these assumptions, the undercooling is given as

$$\Delta T = \sum_{i=1}^{n}\left(c_l^{i*}m_v^i - c_o^i m_o^i\right) - \frac{2\Gamma}{R}, \tag{2}$$

where c_o^i is the nominal composition of the i^{th}element with equilibrium liquid slope m_o^i and velocity-dependent liquidus slope m_v^i. Γ is the Gibbs-Thomson Coefficient, and R the dendrite tip radius [16]. The first term on the right-hand side of Eq. (2) represents the velocity dependent solutal undercooling, and the second term relates to the curvature of the dendrite tip. The liquid concentration of component i at the dendrite tip, c_l^{i*}, is

$$c_l^{i*} = \frac{c_0^i}{[1-(1-k_v^i)Iv(Pe)}, \tag{3}$$

and the velocity dependent liquidus slope is

$$m_v^i = m_0^i\left[\frac{1-k_v^i(1-\ln\{\frac{k_v^i}{k_0^i}\})}{1-k_0^i}\right], \tag{4}$$

where k_v^i is the velocity dependent partition coefficient of component i.

$Iv(Pe) = Pe\exp(Pe)E_1(Pe)$ is the Ivantsov function, which describes the solutal diffusion field ahead of the dendrite by approximating the dendrite tip shape as a paraboloid of revolution, where E_1 is the exponential integral, here calculated using an approximation proposed by Tong and Beckermann [17]. The Ivantsov solution is only a function of the solutal Peclet number, $Pe = V_sR/2D_i$, which describes the ratio of advective transport at the growth velocity V_s, to diffusive transport, governed by the mass diffusivity in the liquid, D_i, over a length scale of the dendrite tip radius, R. The velocity dependent partition coefficient (k_v^i) is calculated using the model of Aziz [18]

$$k_v^i = \frac{k_0^i + \frac{a_0V_s}{D_i}}{1+\frac{a_0V_s}{D_i}}, \tag{5}$$

where a_0 is the lattice parameter.

Lastly, the dendrite tip radius R is calculated according to the KGT