NUMERICAL MODELING OF HEAT-TRANSFER AND THE INFLUENCE OF PROCESS PARAMETERS ON TAILORING THE GRAIN MORPHOLOGY OF IN718 IN ELECTRON BEAM ADDITIVE MANUFACTURING

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Abstract

Additive Manufacturing (AM), the fabrication of 3-D parts from CAD models, is a disruptive technology that is transforming the metal manufacturing industry. The correlation between solidification microstructure and mechanical properties has been well understood in the casting and welding processes over the years. This paper focuses on extending these principles to additive manufacturing to understand the transient phenomena of repeated melting and solidification during electron beam powder melting process to achieve site-specific microstructure control within a fabricated component. In this paper, we have developed a novel melt scan strategy for electron beam melting of nickel-base superalloy (Inconel 718) and also analyzed 3-D heat transfer conditions using a parallel numerical solidification code (Truchas) developed at Los Alamos

National Laboratory. The spatial and temporal variations of temperature gradient (G) and growth velocity (R) at the liquid-solid interface of the melt pool were calculated as a function of electron beam parameters. By manipulating the relative number of voxels that lie in the columnar or equiaxed region, the crystallographic texture of the components can be controlled. The analysis of the parameters provided optimum processing conditions that will result in columnar to equiaxed transition (CET) during the solidification. The results from the numerical simulations were validated by experimental processing and characterization thereby proving the potential of additive manufacturing process to achieve site-specific crystallographic texture control within a fabricated component.

Keywords:

Additive Manufacturing, Nickel-base superalloy, Arcam, Microstructure control, Numerical modeling

1. INTRODUCTION

Additive manufacturing (AM), commonly referred to as rapid prototyping, is the fabrication of 3-D parts by additively fusing one layer of raw material over the previously fused layers. Fabrication of functional parts using AM dramatically reduces material waste compared to conventional subtractive manufacturing processes like machining. During machining, the desired shape and size of the part is obtained by removing the excess material from a large casting or forging. In contrast, during additive manufacturing, the near net shape part is made by melting only the required amount of materials in a controlled fashion. Another advantage of AM over conventional processes is the ability to fabricate geometrically complex structures that are either impossible or expensive through traditional methods like milling and machining.

The majority of metal AM systems fall into two main classifications; powder bed fusion and directed energy deposition. For powder bed fusion systems the starting material is metal powder in contrast to directed energy technologies where the starting material may be either powder or wire. Lasers and electron beams are the two most commonly used heat sources to selectively melt the metal powder particles in the bed and fuse them to the underlying layers. Electron beam based processes have significantly higher power density [1] than laser based processes, and also, the electron beam based Arcam® process has comparatively faster melting rate than laser based processes. Parts fabricated using the electron beam process also tend to have significantly lower residual stresses [2] compared to parts manufactured using laser based fabrication process. Focus of the current research is to explore possibility of achieving on-demand solidification texture within nickel base superalloy components, relevant for energy applications using electron beam additive manufacturing.

Inconel 718 (IN718), a precipitation strengthened nickel-base superalloy is selected for the current study. This alloy has excellent mechanical properties [3], [4] at elevated temperatures, and is being used in gas turbine engines in the aerospace and power generation industries. Traditionally IN718 is used in wrought form, in which subsequent mechanical deformation or post thermal processing is used to create homogeneous isotropic mechanical properties. The metallurgical challenge associated with process of IN718 using additive manufacturing techniques is that the material tends to solidify in an epitaxial manner producing columnar grains with {001} texture oriented along the build direction [5]–[7]. Columnar grains oriented along loading direction are often required for maximizing the high-temperature mechanical performance of parts. At the same time, this anisotropy in mechanical behavior is deemed to be detrimental for applications involving multidirectional stresses. This makes AM an inappropriate choice for fabricating components with isotropic mechanical properties. As a result, ability to attain on-demand crystallographic texture may be relevant for AM processing of single crystal nickel base superalloys typically used in hot sections and equiaxed alloys used in cooler section of the gas turbine engines [8].

Limited studies are available on the crystallographic texture control of IN718 fabricated using electron beam based additive manufacturing. Körner *et al*.[9] shown the possibility of obtaining both epitaxial and near equiaxed grains in different layers by varying the scan strategy and beam parameters between the layers. Dehoff *et al*.[10] experimentally demonstrated the feasibility of producing highly misoriented equiaxed grains and oriented columnar grains in the same layer by rapidly changing the scan strategy between line and point heat sources. The above demonstrations are indeed manifestation of the liquid-solid interface stability and constitutional supercooling during epitaxial solidification affected by spatial and temporal variations of thermal gradient (G) and interface velocity (R) within the molten pool.

Although, control of solidification texture can be achieved by experimental trial and error optimizations, the number of experimental trials can be significantly reduced by using numerical models capable of describing the underlying physics. Recent experimental studies[11]–[13] used infrared thermal imaging techniques to measure the temperature distribution on the surface of the melt pool for microstructural engineering. However, by using numerical simulation of heat transfer and fluid flow, Raghavan *et al.* [14] showed that molten pools with similar top surface temperatures can have significantly different subsurface shapes, resulting in different cooling rates at different locations across the melt pool potentially leading to different microstructures. Shen *et al* [15] developed a numerical thermal model for electron beam AM with multiple cross raster patterns. Cheng *et al.* [16] used the design and analysis of experiments (DOX) [17] approach to derive a relationship between the temperature profile and electron beam parameters. Zäh *et al.* [18] tried to correlate the electron beam speed and power to the size of the melt pool and created an experimental process map to avoid delamination and melt ball formation. Jamshindinia *et al.* [19] compared the effect of pure thermal and thermal-fluid models on the temperature distribution, and also analyzed the effect of powder bed density on the size of the melt pool. All of these studies neither rationalized the microstructure formation nor developed methodologies for site-specific solidification texture. Bontha et al.[20] employed a combined analytical and numerical model to analyze the effect of beam velocity and power on the temperature gradient and growth rate at the liquid-solid interface of the melt pool to understand the columnar to equiaxed transition. Experimental validations were not performed by Bontha et al. [20] and the potential practical difficulties with the proposed high energy density also limit the practicality. Debroy et al. [21]–[24] studied the behavior of temperature distribution, weld pool shape and solidification parameters in single spot welding of steels using numerical simulation of heat transfer and fluid

flow. Furthermore, most of the studies used standard raster scan or energy density and none of them considered alternate strategy. The fundamental question is that, is it possible to design processing conditions to induce grain orientations as demonstrated by Dehoff et al.[10], *a-priori* by numerical experimentations, rather than trial and error experimentation. Therefore, in this study, the physics of heat transfer of point heat source scan strategies in electron beam AM of IN718 is simulated to investigate the effects of various beam parameters on the melt pool dynamics. The spatial and temporal variations of temperature gradient (G) and growth rate (R) at the liquid-solid interface of the melt pool are extracted. Based on this information, the effects of the electron beam input parameters on the fraction of equiaxed grain formation were calculated and experimentally validated. The innovation lies in the development of new melt pattern and reduction of trial and error experimentation for site-specific microstructure control during additive manufacturing.

2. MATHEMATICAL - PHYSICAL MODEL

2.1. Modeling tool

Three dimensional numerical simulations were performed using the code Truchas [25]. Truchas was developed under the Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory (LANL) for simulation of metal casting processes. It is an open-source, continuum scale, multi-physics simulation tool designed to solve large problems on parallel high-performance computing (HPC) platforms. Truchas employs physical models for alloy solidification with heat transfer algorithms accounting for non-isothermal phase change in mushy zones, which is a typical characteristic of complex alloys like IN718.

2.2. Conservation of Energy - Heat Conduction Equation

In Truchas, the heat transfer algorithm uses a local mimetic finite discretization (see Morel *et al* [26] for example) of the Fourier heat conduction **equation (1)**

$$\frac{\partial(\rho h(T))}{\partial t} + \nabla.(k\nabla T) = \dot{Q}(x, y, z) \quad \textbf{(1)}$$

where **ρ** is the mass density, **h(T)** is the enthalpy per unit mass as a function of temperature T, **k** is the thermal conductivity and **T** is the temperature. $\dot{Q}$ represents the volumetric heat source (electron beam) applied to the domain and **∇** is the three dimensional vector differential operator in Cartesian co-ordinates. The enthalpy relation h(T) incorporates the latent heat of phase change. In a single-phase zone, h(T) is defined up to an additive constant by specific heat $C_p = dh/dT$ of the phase. In the two phase mushy zone, h(T) is the mass-weighted average of the h(T) of the individual phases. For this study, the fraction of each phase as a function of T was given by the simple lever rule.

2.3. Heat Source Model

It is important to understand the physics of the interaction of the electron beam with the material in order to model the heat source **($\dot{Q}$)** used in the simulations. The surface heat intensity distribution of electron beam is given by a Gaussian distribution with standard deviation **σ** as formulated in **equation (2)**.

$$I_{xy} = \left(\frac{1}{2\pi\sigma^2}\right) e^{-\frac{1}{2\sigma^2}(x^2+y^2)} \quad (2)$$

Unlike a laser heat source, which interacts only with the surface of the material, an electron beam penetrates significantly into the material thereby creating a heat flux distribution vertically along the z-direction. The electron beam heat flux distribution along the z-direction is formulated in **equation (3)** [18], [19].

$$I_z = -3\left(\frac{z}{z_e}\right)^2 - 2\left(\frac{z}{z_e}\right) + 1 \quad (3)$$

where z_e is the absolute penetration depth of the electron beam into the material where 99% of the beam energy is absorbed. Absolute penetration depth of the electron beam is calculated using **equation (4)** [18], [19].

$$z_e = 2.1 * \left(10^{-5}\right) * \frac{V_e^2}{\rho} \quad (4)$$

where V_e is the electron beam acceleration voltage (kV) and ρ is the density of the material(kg/m-3). **Equation (6)** is obtained by consolidating the **equations (2, 3, 4, 5)** which depicts the mathematical formulation of the volumetric electron beam heat source model used in the simulations.

$$\dot{Q}(x,y,z) = -\eta_e * \eta_b * Q_{max} * \frac{I_{xy} I_z}{z_e} \quad (5)$$

$$\dot{Q}(x,y,z) = -\eta_e * \eta_b * Q_{max} * \frac{4\,ln(0.1)}{\pi * d^2 * z_e} * e^{\left(\frac{4\,ln(0.1)(x^2+y^2)}{d^2}\right)} * \left\{-3\left(\frac{z}{z_e}\right)^2 - 2\left(\frac{z}{z_e}\right) + 1\right\} \quad (6)$$

where η_e, η_b and **d** are energy conversion efficiency on the surface, efficiency of beam control and electron beam diameter respectively. Electron beam energy absorption and beam transfer efficiency are generally in the range of 90% [27] for all the materials. Q_{max} denotes the maximum power of the electron beam which is the product of electron beam current (I_e) and acceleration voltage (V_e) as formulated in **equation (7)**.

$$Q_{max} = I_e * V_e \quad (7)$$

In the Arcam® process, electron beam acceleration voltage is constant (60 kV) and the beam current is a variable.

2.4. Geometry, Meshing and Assumptions

The CUBIT [28] geometry and mesh generation toolkit was used to spatially discretize the domain into structured hexahedral cells of 15 microns along X, Y and Z directions, resulting in a mesh

consisting of approximately 2.7 million nodes. Depending on the number of computational nodes employed, the domain was then subdivided into smaller domains by Truchas using the Chaco partitioning library [29] during the initialization phase of the simulations.

Expansion and shrinkage of the material due to the changes in temperature during melting and solidification were not accounted for in these simulations. The mass was conserved within each cell, and cell volumes were kept constant before, during and after the phase change. Hence, the density of the material was assumed to be constant for all the phases of materials used in the simulation. A computational cycle was allowed to use adaptive time stepping, with a maximum of $1.0x10^{-7}$ and a minimum of $1.0x10^{-10}$ seconds.

2.5. Initial and Boundary Conditions

Local preheat temperature of the substrate, one of the indirect control parameters in Arcam® process, was used as the initial condition of the spatial domain, and was considered a variable in the simulations. The top surface of the build radiates heat to the surroundings. Part fabrication in the Arcam® process takes place in a low pressure environment (10^{-3} mbar partial pressure of helium) [30], therefore the heat transfer due to convection on the top surface of the domain is negligible and was assumed to be zero in the simulations. Hence the boundary condition at the top surface (γ) was formulated by applying energy conservation **equation (8)**

$$-\boldsymbol{k\nabla T} = \boldsymbol{\varepsilon} * \boldsymbol{\sigma} * (\boldsymbol{T_x^4} - \boldsymbol{T_a^4}), \qquad \boldsymbol{x} \in \boldsymbol{\gamma} \tag{8}$$

where $\mathbf{T_a}$ is the ambient temperature, $\mathbf{k}$ is the thermal conductivity of the material, $\boldsymbol{\varepsilon}$ is the emissivity and $\boldsymbol{\sigma}$ is the Stefan-Boltzmann constant.

During the fabrication process, the part is encapsulated by fine metal powder particles of varying diameters (20µ -100µ). Alkahari *et al* [31] experimentally measured and theoretically verified the thermal conductivity of metal powders of varying diameters (10µm -100µm) used in selective laser

melting. The thermal conductivity of metal powders was found to be between 0.33 – 1.5% of the thermal conductivity of bulk metals. The thermal conductivity of metal powders is so low such that it can be considered an insulator for the short duration (milliseconds) of simulations. Hence the boundary conditions on the remaining five faces were assumed to be adiabatic. That is, a Neumann boundary condition with zero flux across the surfaces.

2.6. Material Properties

Thermo-physical properties of solid and liquid phases in IN718, used in the simulations, are given in **Table 1**.

Table 1. Thermophysical properties of IN718 [32], [33]

Property	Value	Unit
Density	7451	kg/m^3
Solidus temperature	1528	K
Liquidus temperature	1610	K
Latent heat of fusion	227000	J/kg
Specific heat capacity of solid	600	J/kg-K
Specific heat capacity of liquid	775	J/kg-K
Thermal conductivity of solid @ 1300 K	26.6	W/m-K
Thermal conductivity of liquid @ 1850 K	29.0	W/m-K

3. SIMULATION: INPUTS, RESULTS AND ANALYSIS

3.1. Input parameters

Grain morphology of metals during rapid solidification processes like electron beam melting depends on local solidification conditions, including the thermal gradient (**G**) and the velocity or growth rate (**R**) at the liquid-solid interface of the melt pool. The availability of numerous controllable input parameters in EBM process means that the control strategy becomes enormous. Based on the prior published literature [10], four process parameters were selected for the comprehensive numerical experimentation.

Table 2 shows the input parameters used in the simulations. The parameter window listed are within the practical limitations of the Arcam® process.

Table 2. Input Parameters

Parameter	Minimum	Maximum
Electron beam Diameter FWHM (μ)	200	800
Electron beam current (mA)	5	20
Spot ON time (ms)	0.1	1
Preheat temperature (K)	973	1528

Spatial and temporal variations of temperature gradient (**G**) at the liquid-solid interface of the melt pool domain are calculated according to **equation (9)**.

$$\boldsymbol{Thermal\ Gradient\ \ G\ (K/m)\ \ =\ \sqrt{G_x^2 + G_y^2 + G_z^2}} \qquad (\mathbf{9})$$

where $\mathbf{G_x}$, $\mathbf{G_y}$ and $\mathbf{G_z}$ are temperature gradients at the liquid-solid interface along X, Y and Z directions respectively. Liquid-solid interface velocity is calculated using cooling rate and temperature gradient as formulated in **equations (10, 11,12)** [34].

$$\boldsymbol{R\ (m/s)\ \ =\ \frac{|Cooling\ Rate|\quad\ (K/s)}{|Thermal\ Gradient|\ \ (K/m)}} \qquad (\mathbf{10})$$

$$\boldsymbol{Cooling\ Rate\ \left(\frac{K}{s}\right)\quad =\quad \left|\frac{dT}{dt}\right|} \qquad (\mathbf{11})$$

$$\boldsymbol{R\ (m/s)\ \ =\ \frac{\left|\frac{dT}{dt}\right|}{\sqrt{G_x^2 + G_y^2 + G_z^2}}} \qquad (\mathbf{12})$$

An analytical model for the columnar to equiaxed transition in casting processes was developed by Hunt [35] which provided relationship between the thermal gradient (**G**), interface velocity (**R**) and volume fraction of equiaxed grains (**Φ**) formed during solidification. Gäumann *et al*. [36] extended the theory using Kurz-Giovanola-Trivedi (KGT) model for rapid solidification processes by neglecting the nucleation undercooling (ΔT_n) at high thermal gradients (~10^6 K/m). The underlying thermodynamics and kinetics of the columnar to equiaxed transition were simplified by Gäumann *et al*. [36] as formulated in **equation (13)**.

$$\left(\frac{G^n}{R}\right) = a\left\{\left(\frac{-4\pi N_o}{3\,ln(1-\Phi)}\right)^{\frac{1}{3}}.\frac{1}{n+1}\right\}^n \quad (13)$$

where **G** is the temperature gradient, **R** is the velocity of the liquid-solid interface, $\mathbf{N_o}$ is the nucleation density, **Φ** is the volume fraction of equiaxed grains or probability of stray grain formation, **n** and **a** are the alloy constants. Nucleation density (**No)** depends on composition of the alloy and undercooling. Higher the value of **No,** higher the probability of formation of equiaxed grains during the solidification. Analytical calculation of the value of **No** is complex and beyond the scope of this paper. In the literature [36]–[38], the value of **No** is experimentally calibrated and optimized. Different values are being reported for the same alloy system [36]–[38]. Values of **a**, **n** and **No** assumed in the results section of this paper are $\mathbf{1.25 \times 10^6}$, **3.4** and $\mathbf{2 \times 10^{15}}$ respectively as reported by Gäumann *et al*. [36] and Vitek [38] for a similar nickel base superalloy. By rearranging **equation** (**13)** and applying the value for constants, the ratio $\mathbf{G^n/R}$ can be directly correlated to the volume fraction of equiaxed or stray grains **(Φ)** formed during the solidification of the melt pool.

$$\Phi = 1 - exp\left\{-2.358E18 * \left(\frac{R}{G^{3.4}}\right)\right\}^{\frac{3}{3.4}} \quad (14)$$

It can be noted from **equation (14)** that the value of **Φ** depends only on the values of **G** and **R**. The calculation of values of **G** and **R** from the numerical simulations is explained in the subsequent section of the paper. In the following section, a qualitative approach of identifying the relative importance of input parameters is shown by plotting spatio-temporal values of **G** and **R** in the reference solidification map [39] of IN718. Quantitative significance of the beam input parameters is studied in the later section of the paper by calculating the volume fraction of equiaxed grains (**Φ**) formed during the solidification of the simulated melt pool.

3.2. Results and Analysis

Figure 1 shows the tracking of the transient liquid-solid interface along XZ symmetrical plane (side view) of a simulated melt pool. In this simulation, the values used for beam current, beam ON time, and preheat temperature of the spatial domain are 20 mA, 1ms and 1528K, respectively. Melting of the substrate continues after the beam is turned off at 1 ms. In this case, the melt pool continues to expand and the solidification begins at 10 ms as shown in **Figure 1(a)** and completely solidifies at 30 ms as shown in **Figure 1(d).**

The thermal gradient (**G**) and cooling rate are calculated at each time step and at each of the voxels in the spatial domain based on **equations (9)** and **(12)**. The calculated values of the temperature gradient and the cooling rate are then filtered along the whole transient liquidus isotherm, to understand the variations along the liquid-solid interface as the solidification proceeds. The direction of the thermal gradient vector is normal to the liquid-solid interface along the liquidus isotherm which essentially dictates the direction of crystal growth at the liquid-solid interface.

Spatial and temporal distributions of the velocity of the liquid-solid interface were then calculated according to **equation (12)**. The values along the liquidus isotherm (1610 K) of the melt pool are used to obtain spatial and temporal distributions of the **G** and **R** only at the liquid-solid interface as the melt pool solidifies. These distributions are then used to predict the transition from columnar to equiaxed microstructure. The extracted **G** and **R** values are plotted on the reference solidification map [39] for IN718.

Figure 2(a) shows the variation of temperature gradient (**G**) and liquid-solid interface velocity (**R**) as the melt pool collapses. From **Figure 2(a)**, it is evident that the temperature gradient is high and the liquid-solid interface velocity is low at the beginning of solidification. As the liquid front

advances and the melt pool shrinks, the temperature gradient decreases and the liquid-solid interface velocity increases rapidly. This transient behavior of G and R with respect to solidification time is in good agreement with the results in spot welding literature [21], [23], [24]. **Figure 2(b)** shows the **G** vs **R** plot on a reference solidification map [39] of IN718. From **Figure 2(b)**, it is evident that grain morphology is columnar as the melt pool begins to solidify and it moves towards mixed region during solidification and results in an equiaxed region at the end of solidification.

Figure 3 shows the spatiotemporal variation of the **G** vs. **R** plot on the solidification map of IN718 for different values of the 4 input parameters with all the other parameters held constant: preheat temperature of the domain (400 K – 1200K), beam ON time (0.1 ms – 1 ms), beam diameter (100 – 600 microns) and beam current (5 – 20 mA) of the point heat source within the practical limitation of the process.

From **Figure 3**, it can be concluded that increasing the preheat temperature, beam current, spot ON time and beam diameter moves the microstructure map towards the equiaxed region from the columnar region by reducing the temperature gradient. Increasing the energy input by increasing the beam power and ON time effectively moves the grain morphology towards the equiaxed region, which is in accordance with the results shown by Bontha *et al* [20]. The sensitivity of the temperature gradient (**G**) and the liquid-solid interface velocity (**R**) with respect to different parameters is shown in **Figure 3**. In order for robust understanding of the columnar to equiaxed transition (CET) during the solidification of the melt pool, it is important to quantify the influence of the beam input parameters (**Table 2)** on **G** and **R**.

Quantitative analysis can be done by calculating the volume fraction of equiaxed grains formed during solidification for different cases of simulated melt pool. The volume fraction of equiaxed

grains, or the probability of stray grain formation (**Φ**), can be calculated at every time step and at every nodal element of spatial domain of the liquid-solid interface using **equation (14)**. The histogram plot in **Figure 4** shows the non-dimensional volume (frequency of nodal elements) vs. the probability of stray grain formation (**Φ**). It can be observed from **Figure 5** that the volume fraction of equiaxed grains in the solidified melt pool can be changed from less than 10% (**Figure 4(a)**) to more than 90% (**Figure 4(b)**) by changing the beam input parameters.

The volume weighted average method formulated in **equation (15)** can then be used to model the stray grain formation in the entire melt pool.

$$\boldsymbol{\Phi} = \frac{\boldsymbol{\Sigma V_i \Phi_i}}{\boldsymbol{\Sigma V_i}} \tag{15}$$

where $\mathbf{V_i}$ is the volume of the discretized nodal element in the spatial domain (dx*dy*dz) and $\mathbf{\Phi_i}$ is the probability of stray grain formation at the corresponding nodal element calculated using **equation (14)**. The design and analysis of experiment (DOX) [17] approach is used to estimate the influence of all the input parameters on the output. A full factorial model is developed with 4 input parameters and 2 levels for each of the factors ($2^k = 2^4$ simulations). The volume fraction of equiaxed grains (**Φ),** calculated using **equation (15),** is used as the response variable in the design. Analysis of variance (ANOVA) approach is used to quantify the effect of each input parameter on the response variable (**Φ)**. The correlation between the input parameters and the response variable is studied in detail.

Simulations were performed for all 16 possible combinations of parameters and weighted volume average of **Φ** is calculated for each of the simulations. The response variable (**Φ)** calculated from the simulations for the statistical design is given in **Table 3**.

Table 3. 2^4 simulation combinations and the corresponding volume fraction of equiaxed grains used in DOX.

Case #	A Beam Diameter (μ)	B Beam Current (mA)	C Spot ON time (ms)	D Preheat Temperature (K)	Response Variable Φ (%)
1	200	5	0.1	973	13.7
2	200	5	0.1	1528	57.5
3	200	5	1	973	15.9
4	200	5	1	1528	75.3
5	200	20	0.1	973	15.8
6	200	20	0.1	1528	67.8
7	200	20	1	973	20.6
8	200	20	1	1528	86.0
9	800	5	0.1	973	14.1
10	800	5	0.1	1528	58.8
11	800	5	1	973	20.4
12	800	5	1	1528	76.9
13	800	20	0.1	973	17.4
14	800	20	0.1	1528	68.2
15	800	20	1	973	22.9
16	800	20	1	1528	88.1

Table 4. Analysis of Variance (ANOVA) of the design

Source	Sum of Squares	Degrees of freedom	Mean Square	F-Value	p-value Probability > F
Model	12904.19	5	2580.84	433.68	< 0.0001
A- Beam Diameter	12.60	1	12.60	2.12	0.1763
B- Beam Current	183.6	1	183.6	30.85	0.0002
C- Beam On Time	538.4	1	538.4	90.45	< 0.0001
D- Preheat Temperature	11979.30	1	11979.30	2012.99	< 0.0001
C*D	190.44	1	190.44	32.00	0.0002

Statistical significance of the individual parameters on the response variable is understood by analyzing the variance (ANOVA) of the design as shown in **Table 4**. The statistical validity of the model is confirmed with the adjusted R-squared value of the design greater than 98%. The significance of each of the input parameters can be explained by their corresponding F-values listed in **Table 4.** The higher the F-value of the parameter, the greater it`s influence on the response variable (**Φ**). Factors with F-value less than 4 are deemed statistically insignificant. The F-values of the parameters indicate that the beam diameter is insignificant (F-value=2.12) and that preheat temperature (F-value = 2012.99) is the most significant in affecting the volume fraction of equiaxed grains (**Φ**) formed during the solidification.

Quantitative relationship between the input parameters and the output response variable (volume fraction of equiaxed grains) is obtained using DOX approach which is formulated in **equation (16).**

$$\boldsymbol{\Phi}\ (\%) = \ \mathbf{-72.07 + 0.4517 * B - 21.6595 * C + 0.083408 * D + 0.027628 * C * D} \qquad (\mathbf{16})$$

where B is beam current (mA), C is beam ON time (ms) and D is the preheat temperature (K). Local preheat temperatures can be maintained high by modifying melt strategies and keeping the entire layer close to the solidus temperature of the alloy. Experimental validation of the same is reported in the following section.

4. EXPERIMENTAL VALIDATION

To validate the modeling results, bulk samples of dimension 2 cm x 2 cm x 2 cm were fabricated with IN718 powder using Arcam® EBM S12 machine. A novel spot melting strategy was developed and used instead of a standard raster melt pattern. The qualitative difference between spot and raster melting is explained in **Figure 5. Figure 5(a)** depicts a standard raster melt pattern in which the electron beam moves linearly to fill the space, as shown by the lines and arrows. **Figure 5(b)** depicts the spot melting pattern used to fabricate the samples to validate the model. In spot melting, the electron beam is turned on at a point with a specified current for a period of time (beam ON time), as indicated in **Table 2**. Once the time period exceeds the defined beam ON time, the beam is moved to a new spot according to the sequence shown in **Figure 5(b)**. Once the entire layer is filled with the independent spots (1-9), the next spot (10) is placed, overlapping the first spot, and the 11th spot is placed beside the 2nd spot, making it independent of the 10th spot, and so on. The spot filling continues in both the horizontal and vertical directions until the entire 2D layer (2 cm x 2 cm) is completely melted. Subsequently, the build platform is lowered and the

melt pattern continues for the next 2D layer. Each layer is 50 microns thick and the samples consist of 400 layers (2 cm) in total.

A total of 16 samples (**Figure 6(a)**) were fabricated with varying beam current (5-20 mA) and beam ON time (0.05–0.25 ms). **Figure 6(b)** shows the corresponding energy deposited (kJ) per layer of the samples.

4.1 Significance of Preheat Temperature

Figure 7 shows the top surface (XY plane) of samples 8 and 16 (in **Figure 6(a)**), that are fabricated using beam currents of 10 and 20 mA, respectively. The beam ON time of 0.25 ms was kept the same for each spot. In the sample fabricated with the beam current of 10 mA (**Figure 7(a)**), it is important to note that the adjacent melt pools are distinct and their solidification are independent of each other. It can be logically inferred that the local preheat temperature of the substrate when electron beam hits spot #10 (see Fig. 5b) is less than the solidus temperature of IN718 (1528 K). But in **Figure 7(b)**, the adjacent melt pools are indistinguishable, which means melt pool #1 does not solidify completely before the electron beam hits spot #10 (see Fig. 5b). This shows that the local preheat temperature of the substrate when electron beam hits spot #10 is greater than or equal to the solidus temperature of IN718 (1528 K). Local preheat temperature of the substrate in the sample 16 is maintained high by depositing more energy per layer (**Figure 6(b))** which keeps the entire layer in molten state before the solidification begins.

The samples 8 and 16 (**Figure 6**) were cut along the build direction (XZ plane) and electron back scattered diffraction (EBSD) imaging was done to determine the crystallographic orientation of the grains. **Figure 8(a)** and **(b)** shows the inverse pole figures of samples 8 and 16 respectively. **Figure 8(c)** and **(d)** shows the corresponding grain aspect ratio map. Directional (columnar) grain growth along the build direction was observed in the sample 8 with distinct melt pools (**Figure**

7(a)). Equiaxed grain growth was observed in the sample 16 with indistinguishable melt pools (**Figure 7(b)**). These experimental results validate the modeling results that local preheat temperature is the most significant factor in columnar to equiaxed transition (CET) during the solidification in the electron beam AM process.

Statistical evidence is provided by corresponding grain aspect ratio maps shown in **Figure 8(c)** and **(d)**. The sample fabricated with beam current of 10 mA has 60% of grains with aspect ratio less than 0.25 while the sample fabricated with beam current of 20 mA has only 6% of grains with aspect ratio less than 0.25.

4.2 Insignificance of Beam Diameter

The significance of beam diameter on grain morphology was experimentally analyzed by fabricating two samples using spot scan strategy (**Figure 5(b)**) with same beam current (20 mA) and beam ON time (1 ms) but different beam diameters. The electron beam in Arcam® is focused using electromagnetic coils, and changing the focus coil current controls the diameter of the beam. Even though the quantitative relationship between focus coil current and beam diameter is unknown, it can be qualitatively determined that larger coil current defocuses the beam, resulting in a larger beam diameter. Samples were fabricated with focus coil currents of 0 mA (highly focused - small beam diameter) and 20 mA (defocused - large beam diameter) within the practical limitation of the process. The samples were fabricated with lower energy deposition (1.9 kJ) per layer in order to decouple the effect of beam diameter from the preheat temperature. Energy deposition was controlled by reducing the number of spots in a layer. Samples were cut along the build direction (XZ plane) and the orientation of the grains were analyzed by studying the EBSD data using a scanning electron microscope. **Figure 9** shows the inverse pole figure along with the corresponding grain aspect ratio of the two samples. In agreement with the results from numerical

simulations, no significant change in grain aspect ratio was observed between the samples. The results in **Figure 8** and **Figure 9** experimentally verify that changing beam diameter has an insignificant effect compared to changing the local preheat temperature of the substrate.

These results are in good agreement with the qualitative conclusions by Gäumann *et al*. [36] and Vitek [38]. Their qualitative conclusion suggested that by using low beam diameter, low beam power and not preheating the substrate, epitaxial growth can be favored thereby avoiding the stray grain (equiaxed) formation during single crystal repair welds. Based on these results, local preheat temperature of the substrate can be increased or decreased by deploying new spot-melt strategies of the electron beam as described and control the grain morphology and texture of the fabricated part. Future research should focus on translating these results to beam or scan control algorithms of additive manufacturing equipment for achieving on-demand site-specific crystallographic texture within complex geometry.

5. SUMMARY AND CONCLUSIONS

Solidification texture of IN718 alloy was controlled during electron beam additive manufacturing by developing a novel melt scanning strategy optimized with a 3-D numerical model capable of predicting the fraction of equiaxed grain formation as a function of beam diameter, beam current, beam ON time, and preheat temperature. The model relies on the spatial and temporal calculation of thermal gradient (**G**) and liquid-solid interface velocity (**R**). The results of these calculations were then coupled with published criteria for columnar to equiaxed transition during solidification.

Using design of experiments principles, numerical evaluations showed that the volume fraction of equiaxed grains (**Φ**) increased, with an increase in beam- diameter, current and –ON time, as well as, preheat temperature. The analysis of variance **(ANOVA)** approach was used to quantify the effect of all the input parameters on the volume fraction of equiaxed grains formed during the

solidification of the simulated melt pool. A quantitative relationship was derived between the input parameters and the volume fraction of equiaxed grains formed. Preheat temperature is found to contribute the most in altering the volume fraction of equiaxed grains formed, and beam diameter is found to be the least significant among all the parameters considered. The influence of each of the beam input parameters on the columnar to equiaxed transition during the solidification was statistically explained.

These calculations, for a given square geometry, yielded optimum spot melting process parameters to induce the columnar to equiaxed transition throughout the bulk of the samples, without trial and error experimentations. These calculations were validated later by experimental processing and microscopy characterization. The current research demonstrates the potential of using computational model to arrive at processing and scan strategies for on demand control of crystallographic texture during electron beam additive manufacturing of nickel base alloys. However, a comprehensive numerical analysis is required to understand the effect of arbitrary sectional geometry and other beam scan strategies on the solidification texture to translate these results for industrial applications.

Acknowledgements

Research was sponsored by the US Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office, under contract DE- AC05-00OR22725 with UT-Battelle, LLC. Research was also sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non- exclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others

to do so, for United States Government purposes. This work was performed, in part, under the auspices of the National Nuclear Security Administration of the US Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396 and supported by the DOE Advanced Simulation and Computing (ASC) program.

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