2016

Feasibility of Attaining Fully Equiaxed Microstructure through Process Variable Control for Additive Manufacturing of Ti-6Al-4V

Sarah Louise Kuntz
Wright State University

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FEASIBILITY OF ACHIEVING FULLY EQUIAXED MICROSTRUCTURE THROUGH PROCESS VARIABLE CONTROL FOR ADDITIVE MANUFACTURING OF Ti-6Al-4V

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering

By

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B.S., Wright State University, 2015

2016
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Abstract
Kuntz, Sarah Louise. M.S.M.E. Department of Mechanical and Materials Engineering, Wright State University, 2016. Feasibility of Attaining Fully Equiaxed Microstructure through Process Variable Control for Additive Manufacturing of Ti-6Al-4V.

One of the greatest challenges in additive manufacturing is fabricating titanium structures with consistent and desirable microstructure. To date, fully columnar deposits have been achieved through direct control of process variables. However, the introduction of external factors appears necessary to achieve fully equiaxed grain morphology using existing commercial processes. This work introduces and employs an analytic model to relate process variables to solidification thermal conditions and expected beta grain morphology at the surface of and at the deepest point in the melt pool. The latter is required in order to ensure the deposited microstructure is maintained even after the deposition of subsequent layers and, thus, the possibility of equiaxed microstructure throughout. By exploring the impact of process variables on thermal, morphological, and geometric trends at the deepest point in the melt pool, this work evaluates four commercial processes, estimates the range of process variables capable of producing fully equiaxed microstructure, and considers the expected size of the resultant equiaxed melt pool.
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1 Introduction

1.1 Motivation

Additive Manufacturing is an alternative manufacturing technique sometimes called 3-D printing. Rather than cutting away excess material, additive manufacturing adds material layer-by-layer until the desired component has been formed. Potential advantages of additive manufacturing include waste reduction, weight optimization and component simplification which contribute to the affordability, strength and endurance of the additively manufactured product [1].

Although early additive manufacturing machines were used almost exclusively for prototyping purposes, recent growth in this field has inspired companies to consider additive manufacturing as a versatile alternative to traditional manufacturing processes [2]. The material under consideration, Ti-6Al-4V, is a particularly important alloy as its biocompatibility and excellent high temperature properties make it desirable for medical and aerospace applications.

In order for additive manufacturing to provide a viable alternative to traditional manufacturing processes, additive manufacturing machines must be able to produce component geometries with consistent and desirable microstructure. While deposits composed solely of columnar beta grains and consisting of a mixture of columnar and equiaxed grains have been attained, fully equiaxed beta grains have not been attained through process parameter control for additive manufacturing of Ti-6Al-4V [3].

Work by Martina, et al. reveals that fully equiaxed microstructure is attainable for additively manufactured Ti-6Al-4V [4]. However, Martina’s work introduces additional steps to the already complex additive process in order to attain fully equiaxed grains. By cold rolling each newly deposited layer, the columnar grains formed at solidification are reshaped into equiaxed grains before another layer of material is added. While effective, this method adds time and complexity to the process. If fully equiaxed microstructure can be attained directly through a combination of process variables resulting in thermal conditions favorable to equiaxed grain growth, this would provide a simpler and more efficient means of achieving fully equiaxed microstructure. The process variables considered herein include absorbed beam power, beam velocity and substrate preheat temperature, all of which can be controlled in the context of commercial additive manufacturing processes.
1.2 Literature Review

Previous researchers in additive manufacturing have employed concepts from welding and casting processes to approximate thermal behavior and grain morphology of additive manufactured metals. Hunt’s criterion boundary curves, originally developed to describe dendrite growth for simple Al-3wt%Cu castings, are a primary example of this.

Hunt’s criterion boundary curves divide the range of possible thermal gradients and solidification rates into three regions: the range of thermal conditions favorable to columnar grain growth, the range of conditions favorable to equiaxed grain growth, and the intermediate region where a mixed morphology is likely to form [5]. The original curves, as published by J. D. Hunt in 1984, are shown below in Figure 1-1.

![Figure 1-1: Hunt's Criterion Curves (Al-3wt%Cu) [5]](image_url)

Although Hunt’s curves were developed for simple casting processes, they provide a qualitative basis for the discussion of more complex solidification problems. In 2003, Kobryn and Semiatin reversed the axes and translated Hunt’s curves from Al-3wt%Cu to Ti-6Al-4V [6]. Specifically, Kobryn adjusted the nucleation parameters within Hunt’s equations until the resulting curves matched experimentally observed morphology regions for Ti-6Al-4V castings and laser glaze specimens [6]. As shown in Figure 1-2, the adjusted curves generally described the morphology regions, allowing for the prediction of grain morphology from thermal gradient and cooling rate. Thus, the utility of Hunt’s criterion curves was determined to extend beyond simple casting processes and to qualitatively describe trends across alloy systems.
Figure 1-2: Solidification Map with Hunt’s Curves and Casting Data (Ti-6Al-4V)

Working collaboratively with Kobryn, Bontha et al. applied Hunt’s curves to additive manufacturing of Ti-6Al-4V in 2003, using them in combination with the Rosenthal solution and finite element modeling (FEM) to predict trends in grain morphology of thin wall and bulky geometry simulations of the LENS™ powder feed process and AeroMet’s Lasform Technology [7].

Derived by Rosenthal in 1946, the 3-D Rosenthal solution was nondimensionalized by Vasinonta et al. in 2000 [8, 9]. This simple solution to the heat transfer equation was first applied to the additive manufacturing for consideration of the LENS process by Dobranich and Dyknuizen of Sandia National Laboratories in 1998 and has since been applied to other commercial additive processes [7, 10-18]. In the context of additive manufacturing, the 3-D Rosenthal solution uses a point heat source to approximate the impact of a laser or electron beam moving across a semi-infinite substrate and provides an equation for temperature as a function of distance from the heat source [15, 18]. Bontha et al. were able to relate changes in process variables (beam power and velocity) to changes in thermal conditions [13, 15]. Finite element modeling conducted by Bontha et al. suggested that the Rosenthal solution provides an accurate prediction of thermal trends and the manner in which thermal properties and solidification microstructure respond to changes in process variables [13-15].

Building on Bontha’s work, Gockel translated the Hunt’s curves for Ti-6Al-4V from the thermal process map (thermal gradient vs. solidification rate) into process space (beam power vs. velocity) using the thermal properties at the surface of the melt pool, as illustrated in Figure 1-3 [3, 19].
Using melt pool data from single bead experimental samples created by NASA Langley’s EBF3, Doak’s 2013 examination of specific sample morphologies confirms that Gockel’s curves provide a basis for the estimation of power and velocity combinations likely to experience equiaxed grain growth [3]. Figure 1-3 shows the sample morphologies plotted on the same axes as Gockel’s translated Hunt’s curves. The percentage beside each data point indicates the fraction of the melt pool, by volume ratio, which displayed equiaxed morphology.

---

1 Comparable to Sciaky Process
While Gockel’s curves reliably indicate the possibility of attaining equiaxed grain morphology at the top surface of the melt pool, Doak’s experimental results indicate that achieving equiaxed grain morphology at the top surface of the melt pool is not equivalent to attaining equiaxed grains throughout the depth of the melt pool. The question arises as to whether the morphology at a single point can be used to predict grain morphology throughout the depth of the melt pool.

Prior work, including Bontha’s exploration of trends in solidification rate and thermal gradient for various process variable combinations, suggests that the thermal conditions required for equiaxed grain growth are first achieved at the top surface of the melt pool [3, 14-16]. As illustrated in Figure 1-5, the thermal gradient increases and the solidification rate decreases with increasing depth in the melt pool, resulting in a shift toward columnar morphology.

Figure 1-4: Translated Hunt’s Curves at Melt Pool Surface in Process Space Plotted with Experimental Data (Ti-6Al-4V) [3]
From inspection of Figure 1-5, if thermal conditions conducive to equiaxed grain growth can be attained at the deepest point of the melt pool, then conditions for equiaxed grain growth should be present for the entire melt pool. If conditions are favorable for equiaxed grain growth throughout the entirety of the melt pool, then equiaxed morphology should also be observed following the deposition of subsequent layers with similar thermal conditions.

Figure 1-5: Impact of Changing Beam Power and Velocity on Thermal Gradient and Solidification Rate throughout melt pool depth (Ti-6Al-4V) [14]
1.3 Approach

As demonstrated by Bontha’s work for the simplest case scenario, that of a single bead formed by a laser glaze or electron beam passing across the surface of a semi-infinite Ti-6Al-4V substrate, achieving equiaxed microstructure at the deepest point in the melt pool should be synonymous with achieving equiaxed microstructure throughout the entirety of the melt pool [14]. This work uses a similar approach to approximate the thermal conditions at the deepest point in the melt pool and to estimate the grain morphology at solidification through comparison with Hunt’s curves for titanium alloy Ti-6Al-4V.

To this end, the analytic model utilized by Bontha was modified for application to the deepest point in the melt pool and a process was developed for systematically applying this approach to a range of process variable combinations. The response of thermal conditions to process variables is compared for the surface of the melt pool2 and the deepest point in the melt pool. Based on the generalized behavior seen in the analytic model, predictions are made regarding the process variable combinations necessary to obtain thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool.

Next, four commercial processes were evaluated via the analytic model to determine whether they may be expected to produce conditions favorable for equiaxed grain growth at the deepest point in the melt pool. The relative size of each process is considered in conjunction with its location relative to Hunt’s criterion boundary curves, and predictions are made regarding the general size of a melt pool expected to experience equiaxed grain growth at its depth.

By iteratively increasing the process preheat condition, a preliminary range of process variables expected to produce fully equiaxed microstructure is defined, tabulated, and presented in graphic form. Additionally, the size of the melt pool, in terms of trailing edge length and melt pool depth, is determined for each of the process variable combinations expected to produce fully equiaxed microstructure.

\[2\text{References to the surface of the melt pool specifically refer to the location at which the trailing edge of the melt pool intersects with the surface of the substrate.}\]
1.4 Material

The material under consideration is the titanium alloy, Ti-6Al-4V. This alloy is of interest in that its excellent high temperature properties and biocompatibility make it ideal for various aerospace and medical applications. As a result, Ti-6Al-4V is perhaps the most extensively researched of the metals currently used in additive manufacturing.

For the Rosenthal-based analytic model, thermophysical material properties are assumed to be independent of temperature. The values used are those from the liquidus temperature, as only the portion of the substrate near the melt pool boundary is of interest. Although material properties change with temperature, they are assumed to be constant for all analytic model computations [8]. The thermophysical properties of Ti-6Al-4V at melting (i.e. liquidus) temperature are provided below in Table 1-1 [7, 16].

Table 1-1: Constants for Ti-6Al-4V

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Name</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_m$</td>
<td>Melting temperature</td>
<td>1654</td>
<td>°C</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Mass density</td>
<td>4002.23</td>
<td>kg/m³</td>
</tr>
<tr>
<td>$c$</td>
<td>Specific heat</td>
<td>857.68</td>
<td>J/kg°C</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal conductivity</td>
<td>30.45</td>
<td>W/m-K</td>
</tr>
<tr>
<td>$T_L$</td>
<td>Liquidus temperature</td>
<td>1654</td>
<td>°C</td>
</tr>
<tr>
<td>$T_S$</td>
<td>Solidus temperature</td>
<td>1620</td>
<td>°C</td>
</tr>
</tbody>
</table>
1.5 Overview and Contributions

In the first part of Chapter 2, the melt pool is introduced in the general context of additive manufacturing and then defined in reference to this work. The remainder of Chapter 2 discusses Bontha’s analytic model and its modification for the deepest point in the melt pool. Exactly how the analytic model is applied to the deepest point in the melt pool is described in Chapter 3. Chapter 4 discusses the impact of process variables upon thermal conditions at solidification and how that impact differs between the surface of the melt pool and its depth (the deepest point in the melt pool). Chapter 5 evaluates four commercial processes as to their ability to produce thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool and utilizes trends in process size to make predictions about the general size expected for a melt pool characterized by thermal conditions favorable for equiaxed grain growth. The first two sections of Chapter 6 build on understanding the response of thermal conditions to process variable changes developed in Chapter 4 to determine a preliminary range of process variables expected to produce fully equiaxed microstructure. The remainder of Chapter 6 provides a process map in terms of absorbed power, velocity and substrate preheat and considers the combined impact of these three variables on melt pool geometry. Chapter 7 contains a summary and suggestions for future work. Next, are the appendices followed by the bibliography. Appendix A contains information regarding Hunt’s Criterion curves, including equations for the curves in terms of thermal gradient and solidification rate. Appendix B features dimensionless curve fit equations relating dimensionless temperature to the ratio of thermal properties at the depth and surface of the melt pool. Appendix C provides sample MATLAB codes for those interested in replicating this work.

The main contributions of this thesis are as follows:

1. Introduces a modified version of Bontha’s analytic model suitable for application to the deepest point in the melt pool
2. Explores the difference between the response of thermal conditions to process variable changes at the depth of the melt pool and at the surface of the melt pool
3. Presents a range of process variables for which equiaxed grain growth at the deepest point in the melt pool may be possible
4. Evaluates four commercial processes based on their projected ability to achieve thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool
5. Examines the impact of process variables on melt pool depth and trailing edge length for the range of process variables likely to produce equiaxed grain growth at the deepest point in the melt pool
2 Background

2.1 Introduction to the Melt Pool

In additive manufacturing, components are formed, layer by layer, through the solidification of molten, deposited material. During this process, the melt pool is defined to be the portion of the material that is melted at a given time. The melt pool is composed of both the added material and the portion of the previous layers that has been re-melted by the laser or electron beam. Figure 2-1 provides an illustration of the melt pool in a multi-layer, added-material setting.

![Melt Pool Illustration](image)

*Figure 2-1: Illustration of Melt Pool for Multilayer Deposition*

In order to determine whether it is possible to attain fully equiaxed microstructure through process variable control, this work considers the simplest scenario in additive manufacturing: that of a single bead on a plate with no added material. The melt pool for this case is illustrated below in Figure 2-2.
Figure 2-2: Illustration of Melt Pool for No Added Material Case

The red arrow indicates the location of the laser or electron beam, generically referred to as the heat source, while the dark gray arrow indicates the direction that the beam is moving. The white region, denoting the melt pool, is the melted region of the Ti-6Al-4V base plate. The violet arrow indicates the depth of the melt pool, as measured from the top surface of the substrate, while the light gray arrow indicates the exact location where maximum depth is reached.

Note that the location of maximum depth (i.e. the deepest point) is not positioned directly beneath the heat source but lags behind it. The leading portion of the melt pool is the melted region occurring before the location of maximum depth, whereas the trailing portion of the melt pool is the region after this point. As a result, the length of the trailing edge is measured horizontally from the deepest point of the melt pool, rather than from the location of the heat source.

The boundary of the melt pool is considered to be the liquidus isotherm, because this is the temperature at which solidification grain growth begins. Thus, the leading edge of the melt pool, traced in green, indicates the location at which the solid titanium substrate completes its transition to liquid phase. The trailing edge, traced in blue, is the location at which the liquid titanium in the melt pool begins its transition back to solid phase.

Note that the coordinate system in Figure 2-2 utilizes relative coordinates \((x_0, y_0, z_0)\), for which the origin translates along the substrate with the melt pool. This is accomplished by defining the origin of the relative coordinate system as the location where the heat source impacts the top surface of the substrate. The positive \(x_0\)-axis lies...
along the top surface of the substrate, coincident with the direction of motion, while the positive $z_0$-axis proceeds vertically into the substrate. The $y_0$-axis is not shown in Figure 2-2, as it points out of the page. For ease of visualization, a three-dimensional representation is provided in Figure 2-3, where a melt pool overlay has been added to Bontha’s semi-infinite bulky, 3-D geometry [15].

![Figure 2-3: Melt Pool Geometry in 3-D, No Added Material](image)

The red triangle, labeled $\alpha Q$, indicates the location of the heat source, while the bold black arrow labeled $V$ defines the direction of motion. The orange region denotes the top surface of the melt pool which lies within the $x_0$- $y_0$ plane. The purple melt pool cross section lies within the $y_0$- $z_0$ plane. The green cross section, lying in the $x_0$- $z_0$ plane, corresponds to the melt pool cross section shown in Figure 2-2 and contains all the melt pool features and measurements of interest in this work.
2.2 3-D Rosenthal Solution

As discussed in Section 1.2, the three-dimensional (3-D) Rosenthal solution has been used, particularly in its dimensionless form, to provide a first order understanding of the relationships between process variables and associated thermal conditions at solidification. Although the solution makes a number of assumptions, the results correspond favorably to the thermal trends seen in additively manufactured titanium [3, 14-16]. As a result, the 3-D Rosenthal solution may be utilized to project the range of process variables likely to produce thermal conditions favorable to equiaxed grain growth at solidification for additively manufactured Ti-6Al-4V.

2.2.1 Rosenthal’s Solution to the 3-D Heat Transfer Equation

In his 1946 work, Rosenthal derived a steady-state solution to the 3-D conduction heat transfer problem. Assumptions inherent to the derivation of Rosenthal’s solution include:

- Temperature independent material properties (c, ρ, k) with no latent heat effects
- A constant point heat source (αQ)
- Constant, linear velocity (V) in the x-direction
- Solid and semi-infinite substrate
- Conduction only (no convection or radiation)

Since velocity is assumed to be linear, constant, and in x-direction, the relative coordinate system is related to the fixed spatial coordinate as

\[(x_0, y_0, z_0) = (x - Vt, y, z)\]  \hspace{1cm} (2.1)

Note that this is the same relative coordinate system introduced in Section 2.1: Introduction to the Melt Pool. Thus, Rosenthal’s solution for pure conduction with a solid is determined to be [8]

\[T - T_0 = \frac{αQ}{2πk} e^{-λVx_0} e^{-λV\sqrt{y_0^2 + z_0^2}} \frac{e^{-λV\sqrt{x_0^2 + y_0^2 + z_0^2}}}{\sqrt{x_0^2 + y_0^2 + z_0^2}}, \text{ where } λ = \frac{αc}{2k} \]  \hspace{1cm} (3-D Rosenthal Solution)  \hspace{1cm} (2.2)

2.2.2 Nondimensionalized 3-D Rosenthal Solution

2.2.2.1 Nondimensionalization

For various thermal fluids problems, nondimensionalization is utilized to obtain a closed form solution that is more widely applicable than the dimensional version would be. Simply put, nondimensionalization simplifies the analysis by allowing a broad range of problems to be considered using the same basic equation, as the nondimensionalization process renders the equation itself independent of size, scale and material, among other factors [20]. Various dimensionless parameters even have physical significance and are known to provide information about the relative behavior of various system factors [21].
Given the applicability and versatility of dimensionless equations, this work utilizes the 3-D Rosenthal solution in dimensionless form for analytic computations. Numeric results are converted to dimensional form for microstructural prediction. The nondimensionalization approach, heavily based upon prior work by Vasinonta and by Bontha, is summarized in Table 2-1 [9, 14, 15].

Table 2-1: Nondimensionalization Approach for 3-D Rosenthal Solution

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Dimensional Notation</th>
<th>Dimensionless Notation</th>
<th>Nondimensionalization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>( t )</td>
<td>( \bar{t} )</td>
<td>( \bar{t} = \left( \frac{\rho c V}{2k} \right) \sqrt{t} )</td>
</tr>
<tr>
<td>Position</td>
<td>( (x_0, y_0, z_0) )</td>
<td>( (\bar{x}_0, \bar{y}_0, \bar{z}_0) )</td>
<td>( (\bar{x}_0, \bar{y}_0, \bar{z}_0) = \left( \frac{\rho c V}{2k} \right) (x_0, y_0, z_0) )</td>
</tr>
<tr>
<td>Temperature</td>
<td>( T )</td>
<td>( \bar{T} )</td>
<td>( \bar{T} = \frac{T - T_0}{\frac{\alpha Q}{\pi k} \left( \frac{\rho c V}{2k} \right)} )</td>
</tr>
<tr>
<td>Thermal Gradient</td>
<td>( G \ or \</td>
<td>\nabla T</td>
<td>)</td>
</tr>
</tbody>
</table>

Material properties \( \rho, c \) and \( k \) are considered to be independent of temperature in accordance with the basic Rosenthal assumptions. Values of \( \rho, c \) and \( k \) at the melting temperature, 1654°C, are provided in Table 1-1: Constants for Ti-6Al-4V. The quantity \( T_0 \) corresponds to the initial temperature of the substrate, also known as substrate preheat temperature. For a system with no process included preheat, \( T_0 \) equals 25°C or room temperature.

The velocity of the heat source, be it laser or electron beam, is represented by \( V \), while \( \alpha Q \) is the amount of heat energy, or power, absorbed by the substrate. For simplicity, \( \alpha Q \) is treated as a single variable—rather than being split into absorption factor, \( \alpha \), and incident power, \( Q \)—and is referred to as absorbed power. All electron or laser beam powers considered in this work are absorbed powers. Unless explicitly stated otherwise, all values are assumed to be in base units (MKS).

The relative nondimensional coordinate system is related to the nondimensional fixed spatial coordinate as:

\[
(\bar{x}_0, \bar{y}_0, \bar{z}_0) = (\bar{x} - \bar{t}, \bar{y}, \bar{z})
\]

---

\(^3\) The nondimensionalization for cooling rate is provided for reference in Section 2.2.3.1. It is not listed here because it is not used to determine cooling rate in this work.

\(^4\) This is equivalent to assuming an absorption factor of \( \alpha = 1 \).
2.2.2.2 Nondimensionalized Equations

Using the nondimensionalization described in the previous section, the 3-D Rosenthal solution is given to be [15]:

$$\bar{T} = e^{-\frac{\left(x_0^2 + y_0^2 + z_0^2\right)}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}} \quad 2.4$$

Differentiation with respect to each relative nondimensional coordinate yields the directional components of nondimensional thermal gradient:

$$\frac{\partial \bar{T}}{\partial x_0} = -\frac{1}{2} x_0 e^{-\frac{\left(x_0^2 + y_0^2 + z_0^2\right)}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}} \left(1 + \frac{x_0}{\sqrt{x_0^2 + y_0^2 + z_0^2}} + \frac{x_0}{x_0^2 + y_0^2 + z_0^2}\right) \quad 2.5$$

$$\frac{\partial \bar{T}}{\partial y_0} = -\frac{1}{2} y_0 e^{-\frac{\left(x_0^2 + y_0^2 + z_0^2\right)}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}} \left(1 + \frac{1}{\sqrt{x_0^2 + y_0^2 + z_0^2}}\right) \quad 2.6$$

$$\frac{\partial \bar{T}}{\partial z_0} = -\frac{1}{2} z_0 e^{-\frac{\left(x_0^2 + y_0^2 + z_0^2\right)}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}} \left(1 + \frac{1}{\sqrt{x_0^2 + y_0^2 + z_0^2}}\right) \quad 2.7$$

The magnitude of thermal gradient, hereafter referred to as the thermal gradient, is obtained from its nondimensional form as described in Table 2-1. The nondimensional thermal gradient is determined in terms of its components as:

$$G = |\nabla \bar{T}| = \sqrt{\left(\frac{\partial \bar{T}}{\partial x_0}\right)^2 + \left(\frac{\partial \bar{T}}{\partial y_0}\right)^2 + \left(\frac{\partial \bar{T}}{\partial z_0}\right)^2} \quad 2.8$$

The second thermal quantity of interest, the solidification rate, is determined from the thermal gradient and cooling rate as:

$$R = -\frac{1}{G} \frac{\partial \bar{T}}{\partial t} \quad 2.9$$

The negative sign renders solidification rate positive for cooling. Thus, a positive value for $R$ corresponds to a positive $x$-direction solidification rate.

---

Note that the quantity referred to as cooling rate is actually the rate of change of temperature with respect to position. As a result, the “cooling rate” is negative when cooling is occurring.
2.2.3 Determining Rosenthal Cooling Rate

2.2.3.1 Dimensionless Cooling Rate Historic Approach

In prior work, cooling rate has been nondimensionalized according to [15] as

$$\frac{\partial T}{\partial t} = \left(\frac{\rho c V}{2k}\right)^2 \left(\frac{\alpha Q V}{nk}\right) \frac{\partial \tilde{T}}{\partial t}$$ \hspace{1cm} (2.10)

where dimensionless cooling rate is given by

$$\frac{\partial \tilde{T}}{\partial t} = \frac{1}{2} e^{-\left(x_0 + \sqrt{x_0^2 + y_0^2 + z_0^2}\right)} \left(1 + \frac{x_0}{\sqrt{x_0^2 + y_0^2 + z_0^2}} + \frac{x_0}{x_0^2 + y_0^2 + z_0^2}\right)$$ \hspace{1cm} (2.11)

Cooling rate values determined using this approach agree reasonably well with values from finite element analysis near the surface of the melt pool ($z_0 = z_0 = 0$) [3, 15, 16]. However, as the melt pool depth increases along the trailing edge, the values determined from Equation 2.10 approach zero, equaling zero at the deepest point in the melt pool.

Mathematically, the dimensionless form of the instantaneous cooling rate is equivalent to the negative of the dimensionless x-direction component of the thermal gradient vector. This may be seen from an examination of Equations 2.5 and 2.11, which are repeated below for ease of reference.

$$\frac{\partial \tilde{T}}{\partial x_0} = -\frac{1}{2} e^{-\left(x_0 + \sqrt{x_0^2 + y_0^2 + z_0^2}\right)} \left(1 + \frac{x_0}{\sqrt{x_0^2 + y_0^2 + z_0^2}} + \frac{x_0}{x_0^2 + y_0^2 + z_0^2}\right)$$ \hspace{1cm} (2.5)

$$\frac{\partial \tilde{T}}{\partial t} = \frac{1}{2} e^{-\left(x_0 + \sqrt{x_0^2 + y_0^2 + z_0^2}\right)} \left(1 + \frac{x_0}{\sqrt{x_0^2 + y_0^2 + z_0^2}} + \frac{x_0}{x_0^2 + y_0^2 + z_0^2}\right)$$ \hspace{1cm} (2.11)

Since there is a linear relationship between time and x-direction position, the similarity is not unreasonable. However, the change in temperature with respect to time in the global context is related to heat dissipation into the substrate as well as the recession of the heat source.

At the surface of the melt pool, cooling mainly occurs in the y-direction as heat source recedes. Toward the depth of the melt pool, more and more heat is dissipated in the $z_0$-direction. Indeed, at the deepest point in the melt pool, nearly all cooling occurs in the $z_0$-direction as the temperature differential is greatest in this direction. Since the dimensionless relative cooling rate of Equation 2.11 is equal to the $x_0$-direction component of the thermal gradient vector, it does not reflect cooling in the $z_0$-direction. For illustrative purposes, the thermal gradient vectors along the boundary of the melt pool are shown in Figure 2-4.
The behavior of this instantaneous cooling rate is analogous to that of velocity in kinematic projectile motion. Just as a vertically launched projectile proceeds upward with a positive but decreasing velocity, so the cooling rate is positive but decreasing along the leading edge of the melt pool and, as the projectile proceeds downwards with a negative but increasing velocity, so the cooling rate is negative but increasing along the trailing edge of the melt pool. As the projectile reaches its maximum height, the y-direction velocity is zero, so the instantaneous cooling rate is zero at the depth of the melt pool. Figure 2-5 provides a visualization of this phenomenon.

![Figure 2-4: Thermal Gradient Vectors along Melt Pool Boundary](image)

![Figure 2-5: Illustration of Relative Rate of Change of Temperature at Melt Pool Depth](image)
2.2.3.2 Approximating Cooling Rate for Global Coordinates

Although the instantaneous cooling rate at the bottom of the melt pool equals zero, neither cooling nor solidification is an instantaneous phenomenon. Rather, solidification at a given node begins when the nodal temperature decreases to the liquidus temperature and continues until the temperature of the substrate reaches the solidus temperature. Thus, solidification cooling rate may be approximated as an average value [7]

\[
\frac{\partial T}{\partial t} \approx \frac{\Delta T}{\Delta t} = \frac{T_S - T_L}{t_S - t_L} \tag{2.12}
\]

where \(T_S\) and \(T_L\) are the solidus and liquidus temperatures, respectively, and \(t_S\) and \(t_L\) are the times at the corresponding nodal temperatures.

According to Equation 2.1 of Section 2.2.1, the relative x-direction coordinate is a function of velocity, time and the global x-direction coordinate,

\[
x_0 = x - V t \tag{2.1}
\]

Solving this equation for time yields

\[
t = \frac{x - x_0}{V} \tag{2.13}
\]

Thus, the time difference \(\Delta t\) from Equation 2.12 may be written in terms of the relative coordinate \(x_0\) as

\[
\Delta t = t_S - t_L = \frac{x - x_{0.S}}{V} - \frac{x - x_{0.L}}{V} = \frac{x_{0.L} - x_{0.S}}{V} = -\frac{\Delta x_0}{V} \tag{2.14}
\]

Substituting this back into Equation 2.12 yields cooling rate as a function of temperature, velocity, and relative position.

\[
\frac{\partial T}{\partial t} \approx -V * \frac{T_S - T_L}{x_{0,S} - x_{0,L}} \tag{2.15}
\]

This implies that if the x-direction distance between the solidus and liquidus isotherms at a given depth is known, then so is the solidification cooling rate. The solidification rate, \(R\), may then be calculated according to Equation 2.9.
3 Implementation of 3-D Rosenthal Solution

3.1 Finding Dimensionless Coordinates of Deepest Point

3.1.1 Explicit Derivative-Based Approach

In order to find the solidification rate and thermal gradient at the deepest point in the melt pool from the Rosenthal-based equations in Section 2.2.2.2, it is necessary to determine the dimensionless coordinates. As mentioned in Section 2.1, the boundary of the melt pool is considered to be the liquidus isotherm and the deepest point in the melt pool is the location on the liquidus isotherm where dimensionless depth, \( \overline{z_0} \), reaches a maximum. The maximum value of a function is typically obtained by taking the derivative of the function, setting the derivative equal to zero, and solving the resultant equation for the depth. Implementing this approach utilizing the partial derivative of dimensionless temperature with respect to dimensionless depth yields the following:

\[
\frac{\partial T}{\partial \overline{z_0}} = 0 \Rightarrow \left\{ \begin{array}{l}
\text{Case A:} & \overline{z_0} = 0, \text{where} \ \overline{y_0}^2 + \overline{z_0}^2 \neq 0 \\
\text{Case B:} & e^{-\left(\frac{x_0+\sqrt{x_0^2+y_0^2+z_0^2}}{x_0^2+y_0^2+z_0^2}\right)} \left(1 + \frac{1}{\sqrt{x_0^2+y_0^2+z_0^2}}\right) = 0
\end{array} \right. \] 3.1

Since Case A corresponds to the top surface of the melt pool, the solution for maximum depth must lie within Case B. As Case B cannot be solved explicitly, the solution must be determined numerically. The approach detailed in the following section is a modification of the iterative methodology seen in the appendices of [7] and [16].

3.1.2 Iterative Geometry-Based Approach

To numerically determine the dimensionless coordinates for the depth of the melt pool, the liquidus temperature is set equal to the Rosenthal solution in dimensionless form:

\[
\overline{T_m} = \frac{T_L - T_0}{\left(\frac{\alpha q}{\pi k}\right)\epsilon V} = \frac{-\left(x_0+\sqrt{x_0^2+y_0^2+z_0^2}\right)}{2 \sqrt{x_0^2+y_0^2+z_0^2}} \] 3.2

Although simpler than the derivative-based approach from the previous section, Equation 3.2 cannot be solved explicitly. It can, however, be simplified through an understanding of melt pool geometry.

For a uniform substrate, the melt pool is assumed to be symmetric about the \( \overline{x_0}-\overline{z_0} \) plane, as visualized in Figure 2-3 from Section 2.1 (replicated below for convenience). The green cross section corresponds to the plane and the magenta star marks the projected location of the deepest point. Note that the deepest point lies upon the plane of symmetry, \( \overline{x_0}-\overline{z_0} \); thus the \( \overline{y_0} \)-coordinate of the deepest point is zero.
Figure 3-1: Melt Pool Geometry in 3-D, Dimensionless Coordinates [15]

Setting \( \overline{y}_0 \) equal to zero simplifies Equation 3.2 to:

\[
\overline{T}_m = \frac{e^{-\left(\overline{x}_0 + \sqrt{\overline{x}_0^2 + \overline{z}_0^2}\right)}}{2\sqrt{\overline{x}_0^2 + \overline{z}_0^2}} \tag{3.3}
\]

This equation can be used in conjunction with a numerical root finder to solve for either \( \overline{x}_0 \) or \( \overline{z}_0 \), given an initial guess as to the size of the quantity solved for and a fixed value for the alternate variable. That is, in order to find the \( \overline{x}_0 \) coordinate, the \( \overline{z}_0 \) coordinate must be known. The reverse also applies: in order to find the \( \overline{z}_0 \) coordinate, the \( \overline{x}_0 \) coordinate must be known.

A vector of \( \overline{z}_0 \) values was created, ranging from the top of the substrate (\( \overline{z}_0 = 0 \)) to the nondimensionalized melt pool depth (\( \overline{z}_0 = \overline{d} \)). Using the nondimensional length measurement as an initial guess, the \( \overline{x}_0 \) value corresponding to the trailing edge was computed for the top of the melt pool (\( \overline{z}_0 = 0 \)). For each of the subsequent depths, the previous value of \( \overline{x}_0 \) was used as the initial guess. Once a value of \( \overline{x}_0 \) was determined for each incremental depth \( \overline{z}_0 \), the thermal gradient, cooling rate, and solidification rate were computed. Figure 3-2 provides a visual illustration of this process where the purple dots correspond to varying values of \( \overline{z}_0 \) and the green dots correspond to the resulting \((\overline{x}_0, \overline{z}_0)\) pairs. The quantity \( \overline{d} \) is the dimensionless depth obtained from experimental measurements. Note that \( \overline{x}_0 \) values along the trailing edge are negative.\(^6\)

\(^6\) This description corresponds to the iterative approach seen in Bontha’s and Davis’s work from the MATLAB code provided in their appendices [7, 16]
3.1.2.1 Determination of Initial Guesses

Starting from a set of values provided by Davis, an iterative model was created to fabricate initial guesses for both the dimensionless melt pool depth, $\bar{d}$, and the nondimensionalized length measurement, $\bar{\ell}$, used to find $\bar{x}_0$ for the top surface of the melt pool [16]. These initial values are provided below in Table 3-1 for reference. Note that the nondimensionalized length measurement, $\bar{\ell}$, is reported as being negative, since it is measured in the negative $\bar{x}_0$-direction.

Table 3-1: Published Values from Prior Work for a Single Iterative Case [16]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha Q$</td>
<td>Absorbed power (W) $^7$</td>
<td>122.5</td>
</tr>
<tr>
<td>$V$</td>
<td>Beam velocity (in/min)</td>
<td>20</td>
</tr>
<tr>
<td>$T_0$</td>
<td>Preheat temperature (oC)</td>
<td>25</td>
</tr>
<tr>
<td>$\bar{d}$</td>
<td>Dimensionless depth</td>
<td>0.065065</td>
</tr>
<tr>
<td>$\bar{\ell}$</td>
<td>Dimensionless length (initial guess)</td>
<td>$-0.079234$</td>
</tr>
</tbody>
</table>

Sheridan’s 2016 work provides a direct relationship between the initial guess $\bar{\ell}$ and the quantity $\bar{T}_m$ [22]:

$$\bar{\ell} = -\frac{1}{2 \bar{T}_m} \quad \text{(3.4)}$$

Since $\bar{T}_m$ is known for a given power velocity combination, the only remaining unknown is dimensionless depth. The MATLAB code, provided in Appendix C-2, utilizes a series of conditional statements to numerically calculate dimensionless depth.

$^7$ Q=350W, $\alpha=0.35$
4 Response to Process Variable Changes in Melt Pool at Depth and Surface

4.1 Changing Absorbed Power and Velocity

The general response of thermal conditions at the deepest point in the melt pool to changes in beam power and velocity is quite different than that seen at the melt pool surface. The behavioral trends agree with the trends observed from Bontha’s solidification maps [7, 15]. Thermal conditions favorable to equiaxed grain growth are attainable at the surface of the melt pool for lower powers and a wider range of velocities, as compared to the deepest point in the melt pool. This phenomenon is illustrated below in Figure 4-1.

Each color corresponds to a specific beam velocity while each symbol denotes a specific beam power. Points corresponding to a single power are connected by gray lines while points corresponding to a single velocity are connected by lines that match the color assigned to that velocity. At the top of the melt pool (Figure 4-1(a)), the lines of constant power are horizontal while the lines of constant velocity are vertical. However, at the deepest point in the melt pool (Figure 4-1(b)) the lines of constant power curve upward to the right, while the lines of constant velocity curve downward to the left. A legend is provided in the bottom right hand corner of Figure 4-1(b), which applies to Figure 4-1(a) as well.

![Graphs showing impact of changing power and velocity on thermal trends at the surface and 99% depth of the melt pool.](image)

Figure 4-1: Comparison of Thermal Behavior at the Top and Bottom of the Melt Pool

At the top of the smelt pool, increasing velocity corresponds to an increase in solidification rate. Similarly, an increase in beam power corresponds to a decrease in
thermal gradient. Changing the velocity does not impact the thermal gradient. Changing the power does not impact the solidification rate.

In contrast, at the deepest point in the melt pool, both thermal gradient and solidification rate respond to changes in power and velocity. Increasing power still corresponds to a decrease in thermal gradient, and increasing velocity to an increase in solidification rate. However, an increase in power also corresponds to a decrease in solidification rate. This decrease is negligible for low-power-velocity combinations, but becomes noticeable, particularly for high powers, as velocity increases. Similarly, an increase in velocity corresponds to an increase in thermal gradient. Again, this increase is negligible for low-power-velocity combinations but becomes increasingly pronounced, particularly at high powers, as velocity increases.

Although approximately 1/3 of the power and velocity combinations considered in Figure 4-1 are expected to produce thermal conditions favorable for equiaxed grain growth at the surface of the melt pool, none of the process variable combinations are expected to produce thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool.

### 4.2 Changing Velocity and Substrate Preheat

An additional process variable, substrate preheat\(^8\), is varied between 25°C and 1600°C in Figure 4-2 below for a representative power of 500 W and the same range of velocities considered in Figure 4-1. Each color corresponds to a specific beam velocity while each symbol denotes a different preheat temperature. Points corresponding to a given preheat are connected by gray lines while points corresponding to a single velocity are connected by lines that match the color assigned to that velocity. In general, the lines of constant preheat are horizontal while the lines of constant velocity are vertical. This is explicitly true at the top of the melt pool (Figure 4-2(a)), while the behavior at the bottom (Figure 4-2 (b)) is more complex. A legend is provided in the bottom right hand corner of Figure 4-2(b) which applies to Figure 4-2(a) as well.

---

\(^8\) Also known as process preheat
For the surface of the melt pool, the impact of preheat temperature is remarkably similar to that of beam power, as discussed in the previous section. Increasing preheat corresponds to a decrease in thermal gradient. However, there is some slight variation observed in the solidification rate at the surface of the melt pool for the highest preheat considered. Here, the solidification rate decreases slightly in response to the increase in preheat temperature.

As for the bottom of the melt pool, increasing preheat temperature corresponds to a decrease in thermal gradient. Unlike the impact of increasing power, the impact of each change in preheat temperature appears to correspond to a relatively fixed change in thermal gradient. This is of particular interest at the higher velocities where the impact of increasing beam power on the thermal gradient diminishes (see Figure 4-1). The impact of increasing preheat on solidification rate is rather more complex. For the first two velocities considered (0.05 and 0.5 mm/s), increasing preheat temperature corresponds to an increase in solidification rate. For the remaining velocities, increasing preheat temperature corresponds to a decrease in solidification rate. The relative rate of change appears to be slightly greater for 0.05 mm/s (blue) than for 0.5 mm/s (violet) among the first two velocities considered. For the remaining velocities, the magnitude of the impact on solidification rate appears to increase with velocity.

Note that combining a preheat temperature of 1500°C (~90% of the liquidus temperature) with a velocity of 0.5, 5 or 10 mm/s is projected to result in thermal conditions favorable for equiaxed grain growth at the depth of the melt pool for a beam power as low as 500W. This implies that equiaxed grain growth should be possible at the deepest point in the melt pool if only for very high preheat temperatures.
4.3 Changing Absorbed Power, Velocity and Preheat

The solidification map illustrating the impact of changing beam power and velocity on thermal gradient and solidification rate at the deepest point in the melt pool from Figure 4-1(b) is replicated below as Figure 4-3(a). The same range of beam powers and velocities are considered in Figure 4-3(b) using a preheat temperature of 750°C rather than 25°C (no preheat). Once again, each color used corresponds to a specific beam velocity while each symbol denotes a specific beam power. Points corresponding to a single power are connected by gray lines while points corresponding to a single velocity are connected by lines of the color assigned to that velocity.

While both Figure 4-3(a) and Figure 4-3(b) consider the same range of beam powers and velocities, the thermal gradients in Figure 4-3(b), corresponding to a 750°C preheat, are generally lower than those seen for Figure 4-3(a). There is no clear impact on solidification rate behavior, which is not surprising given that the solidification rate effects seen in Figure 4-2 were relatively small, even for very high preheat temperatures. Further, a few of the power-velocity combinations seen in Figure 4-3(b) (750°C preheat) fall in the mixed morphology region, whereas all of the power-velocity combinations seen in Figure 4-3(a) (no preheat) fell in the columnar region. This indicates that the introduction of a substrate preheat is sufficient to alter thermal gradients and, thus, grain morphology. If these trends hold and a high enough substrate preheat is used, thermal conditions favorable to equiaxed grain growth should be attainable at the deepest point in the melt pool.

---

9 750°C is about 45% of the liquidus temperature ($T_L$)
4.4 Summary of General Trends

The response of thermal trends to changes in process variables is different for the deepest point in the melt pool than for the surface of the melt pool. These differences make it unlikely that thermal conditions favorable to equiaxed grain growth will be attained at the deepest point in the melt pool for any beam power and velocity combination with no process preheat (substrate temperature 25°C). Adding a process preheat results in a net decrease in thermal gradient with minimal impact on solidification rate. If a high enough preheat temperature is used in conjunction with a low velocity (0.5-10 mm/s) and an appropriate absorbed beam power, conditions favorable to equiaxed grain growth are predicted for the deepest point in the melt pool. The feasibility of this will be explored further in an upcoming section.
5 Consideration of Four Commercial Processes

5.1 Introduction to the Processes

Having determined the range of process variable combinations for which thermal conditions favorable to equiaxed grain growth are likely to occur, it is relevant to consider existing commercial processes and assess the likelihood of achieving thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool.

Four representative commercial processes, Optomec LENS, Sciaky, EOS and Arcam, are evaluated according to the process variable specifications listed on their respective websites. Figure 5-1 summarizes the range of beam powers and velocities reported for each process. In general, laser-based processes, such as LENS, have an absorption factor on the order of 0.35, while the expected absorptivity for electron-beam based processes is much higher [14, 15, 23-25]. Since beam absorptivity varies among the processes considered, as well as among individual machines within each process, all beam powers are treated as absorbed powers for simplicity’s sake. This means that the maximum power considered for each process is greater than or equal to that which can be obtained experimentally. Since increasing power tends to decrease thermal gradient, the minimum thermal gradients shown for each process are less than or equal to the minimum thermal gradient values that would result if beam absorptivity were taken into account.

Note that the Arcam process utilizes a substrate preheat temperature between 600 and 1000°C [26]. Preheat is not displayed in Figure 5-1 as the LENS, Sciaky and EOS processes do not preheat the substrate (effective preheat of 25°C).
5.2 Thermal Conditions at Melt Pool Depth for Each Process

Using the methodology developed in Chapters 2 and 3, the thermal conditions at the deepest point in the melt pool were obtained for a range of beam powers and velocities corresponding to the capabilities of each process. For each of the powers listed in Table 5-1, the thermal conditions were determined at each of the velocities listed for that process in Table 5-2 using a preheat temperature of 25°C. The Arcam process was also considered using preheat temperatures of 750°C and 1000°C.

Table 5-1: Specific Powers Considered for Each Process in Watts

<table>
<thead>
<tr>
<th>LENS</th>
<th>EOS</th>
<th>Sciaxy</th>
<th>Arcam</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>50</td>
<td>1000</td>
<td>50</td>
</tr>
<tr>
<td>400</td>
<td>75</td>
<td>5000</td>
<td>100</td>
</tr>
<tr>
<td>500</td>
<td>100</td>
<td>10,000</td>
<td>250</td>
</tr>
<tr>
<td>1000</td>
<td>200</td>
<td>20,000</td>
<td>500</td>
</tr>
<tr>
<td>2000</td>
<td>300</td>
<td>30,000</td>
<td>1000</td>
</tr>
<tr>
<td>3000</td>
<td>400</td>
<td>42,000</td>
<td>2000</td>
</tr>
<tr>
<td>4000</td>
<td>500</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 5-2: Specific Velocities Considered for Each Process

| Velocities for | Velocities for |
| LENS & Sciaky | EOS & Arcam |
| in/min | mm/s | in/min | mm/s |
| 0.1 | 0.0423 | 100 | 41.7 |
| 1 | 0.423 | 250 | 104 |
| 10 | 4.17 | 500 | 208 |
| 25 | 10.4 | 750 | 313 |
| 50 | 20.8 | 1000 | 417 |
| 100 | 41.7 | 1500 | 625 |
| 2500 | | 2500 | 1041.67 |

Figure 5-2 below plots the thermal conditions expected at the deepest point in the melt pool for the process variable combinations corresponding to each of the four processes. Since Arcam is the only process of those considered to employ at process preheat condition, it is considered at three different preheat temperatures: 1000°C (maximum Arcam preheat temperature), 750°C preheat and 25°C (no preheat). The no-preheat conditions is primarily for comparison’s sake as the Arcam process cannot function without a preheat condition.

Figure 5-2: Solidification Map at Deepest Point in the Melt Pool for Four Commercial Processes

Sciaky: 1 – 40 kW, 0.04 – 42 mm/s
LENS: 100 – 500 W, 0.04 – 42 mm/s
EOS: 50 – 500 W, 42 – 1060 mm/s
Arcam: 50 – 2000 W, 42 – 1060 mm/s
Arcam: 50 – 2000 W, 42 – 1060 mm/s
Arcam: 50 – 2000 W, 42 – 1060 mm/s
The thermal conditions expected at melt pool depth lie in the columnar morphology region for all process variable combinations considered. This is not surprising, since these processes have not historically produced equiaxed grain growth throughout the depth of the melt pool.

This prediction also agrees with the trends discussed in Chapter 4. Thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool are not expected for any power-velocity combination in the absence of a process preheat condition. While adding a process preheat makes it theoretically possible to obtain thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool, the preheat must be above 1000°C, the maximum Arcam preheat temperature. As a result, none of these four processes are expected to achieve fully equiaxed microstructure through process variable control.

### 5.3 Relative Melt Pool Size

Although these four commercial processes are not expected to be able to obtain equiaxed grain growth at the deepest point in the melt pool through process variable control alone, the relative location of each process on the Figure 5-2 solidification map is instructive. A consideration of Figure 5-2 of the previous section reveals that the Sciaky range of process variables comes closest to Hunt’s criterion boundary curves for a power of 40 kW power and a velocity of ~5 mm/s.

This suggests that the preheat temperature necessary to achieve thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool for power-velocity combinations on this order will be small compared to the preheat temperature required for other power-velocity combinations. As a result, it is instructive to consider the relative scale of these four commercial processes in order to understand the relative melt pool size for which a comparatively low process preheat temperature is expected to generate thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool. Figure 5-3 shows the relative scale of each process by displaying the melt pool contour of a representative power and velocity combination from each of the four processes. Notice that the Arcam 750°C preheat case is included in blue, while the same power and velocity combination with no preheat is represented in black.
Figure 5-3: Melt Pool Contours for Representative Process Variable Combinations

(a) Melt pool contours for representative points  (b) Representative process points

Note that the Arcam 750°C preheat case features a slightly deeper and more elongated melt pool than that seen for the no preheat case.

If this trend holds, then a process utilizing a Sciaky-range power and velocity combination with a relatively low preheat would generate a melt pool of similar size to that shown for Sciaky but be slightly deeper and notably longer. Since the Sciaky melt pool contour is the largest of all four processes, on the order of 3 cm long by 1 cm in depth, it seems logical that a process capable of achieving conditions favorable for equiaxed grain growth at the deepest point in the melt pool using a relatively low process preheat would produce a similarly large melt pool. A more detailed consideration of the combined impact of absorbed beam power, beam velocity and process preheat on melt pool geometry is provided in Section 6.4: Melt Pool Size Predictions for Equiaxed Grain Growth.
6 Process Variable Combinations Involving Elevated Substrate Preheat Temperatures

6.1 Preheat Temperatures Up to 1000°C

Due to the interconnected response of thermal gradient and solidification rate to changes in absorbed power and beam velocity, no power-velocity combination is expected to generate thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool for the case of an unheated substrate (initial substrate temperature 25°C). However, introducing a process preheat condition lowers the thermal gradient for a given power-velocity combination without substantially impacting the solidification rate. As the 750°C preheat condition from Chapter 4, Section 4.3, only achieved thermal conditions sufficient to obtain a mixture of columnar and equiaxed grains at the deepest point in the melt pool, higher substrate preheat temperatures must be considered in order to obtain thermal conditions likely to produce only equiaxed grain growth.

As 750°C is approximately 45% of liquidus temperature for Ti-6Al-4V, the next logical temperature to consider is 850°C, which is approximately 50% of the liquidus melt temperature. The thermal conditions predicted for a range of power and velocity combinations are shown below in Figure 6-1.

![Figure 6-1: Solidification Map for Power and Velocity Combinations at 50% of Liquidus Temperature (850°C)](image-url)
While an improvement over the 750°C preheat case, preheating the substrate to 850°C (50% of liquidus temp.) is insufficient to achieve thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool. Using the maximum Arcam preheat temperature, 1000°C (60% of liquidus), is an improvement upon the previously considered preheat temperatures but it is still insufficient to produce thermal conditions favorable for equiaxed grain growth, as shown in Figure 6-2, below.

![Impact of Changing Power & Velocity on Thermal Trends at Melt Pool Depth with 1000°C Preheat](image)

**Figure 6-2: Solidification Map for a Range of Power and Velocity Combinations at Maximum Arcam Preheat Temperature (1000°C)**

### 6.2 Preheat Temperatures above 1000°C

By iteratively increasing the substrate preheat temperature for a range of absorbed powers and velocities, it is possible to estimate the magnitude of the required preheat temperature. Increasing by 100°C increments from 1000°C, a 1300°C preheat temperature (~80% of liquidus temperature) is the first to yield thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool. Figure 6-3 illustrates the predicted grain morphology at melt pool depth for a range of beam powers and velocities using the preheat conditions of 1100°C and 1200°C while Figure 6-4 illustrates the same for the 1300°C preheat condition.
Figure 6-3: Solidification Map for Power and Velocity Combinations at 1100°C and 1200°C

For the 1300°C substrate preheat, two of the eight velocities considered and three of the absorbed powers are predicted to produce the desired thermal conditions at the
The deepest point in the melt pool. The first of the two velocities, 5 mm/s, has the widest range of acceptable powers: 50 kW, 75 kW and 100 kW. For the second velocity, 10 mm/s, only the 75 kW and 100 kW powers fall in the equiaxed region. Although these absorbed beam powers are higher than those used by the four commercial processes considered, this power-velocity range is consistent with that predicted in Section 5.3. The highest power considered for the Sciaky process was 40 kW and the velocity that produced thermal conditions closest to Hunt’s criterion boundary curves was ~5 mm/s. This indicates that a relatively low preheat temperature capable of producing thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool will be on the order of 80% of the melt pool temperature.

Increasing the preheat temperature to 1400°C (~85% of liquidus temperature) widens the range of possibilities. As shown in Figure 6-5, five of the eight velocities and four of the absorbed powers yield thermal conditions in the equiaxed region. The lowest absorbed beam power required for the 1400°C case is 10 kW. While still beyond the capability of the LENS, EOS and Arcam processes, this power is well within the range of the Sciaky process.

![Impact of Changing Power & Velocity on Thermal Trends at Melt Pool Depth with 1400°C Preheat](image)

**Figure 6-5: Solidification Map for Power and Velocity Combinations at 1400°C**

Increasing the preheat temperature to 1500°C (~90% of liquidus temperature) further decreases thermal gradient values, again with minimal impact on solidification rate as
shown below in Figure 6-6. For this preheat temperature, all the velocities considered, with the exception of 0.05 mm/s, can be utilized to create thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool. The minimum absorbed power required is reduced to 500 W, which is well within the spectrum of commercially used laser and electron beams.

Figure 6-6: Range of Power and Velocity Combinations at 1500°C Preheat
6.3 Process Variables for Equiaxed Grain Growth

The previous section illustrates that thermal conditions favorable to equiaxed grain growth should be attainable at melt pool depth at specific power and velocity combinations corresponding to preheat temperatures 1300°C, 1400°C and 1500°C (~80%, ~85% and ~90% of the liquidus temperature, respectively). These preheat temperatures, along with six others ranging from 76% to 94% of the liquidus temperature, are considered below in Figure 6-7.

Each point plotted represents a single power and velocity combination. Each color corresponds to a different preheat temperature, as specified in the legend. The boundary of each power-velocity-preheat region is outlined in the color corresponding to that preheat for ease of visualization; functions do not exist for these curves. Note, also, that this plot uses the base-ten logarithmic scale on both axes due to the wide range of velocities and powers considered.

![Figure 6-7: Range of Power and Velocity Combinations Predicted to Yield Thermal Conditions Favorable to Equiaxed Grain Growth at Melt Pool Depth for Various Preheat Temperatures](image)
Preheat temperatures higher than 1550°C (94% of the liquidus temperature) may be used in conjunction with lower absorbed beam powers to achieve thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool.

### 6.4 Melt Pool Size Predictions for Equiaxed Grain Growth

As the substrate preheat temperature approaches the liquidus melt temperature, melt pool size increases for a given power-velocity combination. When the substrate preheat equals the liquidus temperature, the entire substrate has melted, resulting in a casting, rather than an additively applicable melt pool. Thus, the concern arises that preheat temperatures near the liquidus melt temperature may result in unusably large melt pools. This section considers the expected melt pool dimensions for each of the process variable combinations considered in the previous section (Figure 6-7).

#### 6.4.1 Four Melt Pool Contours: Comparison with Sciaky Melt Pool

Figure 6-8(a) considers four melt pool contours plotted on the same axes. The dark red melt pool corresponds to the representative Sciaky case considered in Chapter 5, while the bright red, yellow, and orange melt pools correspond to specific elevated preheat cases. Figure 6-8(b) indicates where the power-velocity-preheat conditions lie on the power-velocity-preheat map introduced as Figure 6-7 of Section 6.3. Note that no point corresponding to the representative Sciaky melt pool appears in Figure 6-8(b), as Figure 6-8(b) only displays process variable combinations expected to produce thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool.

If melt pool size increased with preheat temperature, irrespective of changes in power and velocity, the melt pool contours of Figure 6-8(a) would all be larger than the Sciaky contour which has no preheat. Since this is not the case, changes in process preheat do not eliminate the impact of beam power and velocity on melt pool geometry. As a result, conclusions about the relative size of a high preheat temperature melt pool cannot be drawn from knowledge of the preheat temperature alone.
6.4.2 Investigation of Melt Pool Size for Near-Melt-Temperature Preheats

For each of the power-velocity-preheat combinations shown in Figure 6-7 of Section 6.3, melt pool depth and the length of the melt pool trailing edge\textsuperscript{11}, in centimeters, were considered in order to qualitatively measure melt pool size for comparison with the four commercial processes. Like solidification rate and thermal gradient at the deepest point in the melt pool, the depth of the melt pool and the trailing edge length varied in response to changes in absorbed power, velocity and preheat temperature. The dimensionless melt temperature, $\overline{T}_m$, introduced in Section 3.1.2, takes into account all three of these process variables.

Figure 6-9 shows the trailing edge length of the melt pool plotted against the dimensionless melt temperature while Figure 6-10 shows the depth plotted against the dimensionless melt temperature. As in Figure 6-7 of Section 6.3, each point plotted represents a single power-velocity combination and each color corresponds to a different preheat temperature, as specified in the legend. Recall that only power-velocity-preheat combinations expected to generate thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool are considered. Again, the boundary of each power-velocity-preheat region is outlined in the color corresponding to that preheat for ease of visualization as functions do not exist for these curves.

\footnotetext{11}{The length of the melt pool trailing edge as defined in Section 2.1: Introduction to the Melt Pool and is calculated as the absolute value of the difference between the xL at the surface and xL at the depth of the melt pool.}
Figure 6-9: Melt Pool Trailing Edge Length vs. $\overline{T_m}$ for a Range of Power-Velocity-Preheat Combinations

Note that the power-velocity combinations are arranged in a lattice. The horizontal (or pseudo-horizontal, in some cases) rows correspond to a single power. As power increases, so does the melt pool trailing edge length. The rows that ascend to the left at an angle of approximately seventy degrees ($70^\circ$) correspond to lines of constant velocity. Since changes in velocity are primarily horizontal shifts, the primary variable impacting melt pool trailing edge length is absorbed power. Changes in substrate preheat temperature primarily provide a limiting factor regarding the range of powers and velocities expected to produce thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool.
Figure 6-10: Melt Pool Depth vs. $T_m$ for a Range of Power-Velocity-Preheat Combinations

Here, as well, the power-velocity combinations are arranged in a lattice. The rows that ascend to the right along a slightly curved trajectory correspond to lines of constant power. The rows that ascend to the left at an angle of approximately forty degrees ($40^\circ$) correspond to lines of constant velocity. For a constant velocity, increasing the absorbed power increases the depth of the melt pool. For a constant power, increasing the velocity decreases the depth of the melt pool. Since both absorbed power and velocity change diagonally, it is possible, by adjusting power, to maintain the same melt pool depth for different velocities. Similarly, it is possible, by adjusting the beam velocity, to maintain the same melt pool depth for different powers. The primary impact of substrate preheat temperature is, again, to provide a limiting factor regarding the range of powers and velocities expected to produce thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool.
7 Summary and Conclusions

7.1 Outline of Contributions

The main contributions of this thesis are as follows:

1. Introduces a modified version of Bontha’s analytic model suitable for application to the deepest point in the melt pool
2. Explores the difference between the response of thermal conditions to process variable changes at the depth of the melt pool and at the surface of the melt pool
3. Presents a range of process variables for which equiaxed grain growth at the deepest point in the melt pool may be possible
4. Evaluates four commercial processes based on their projected ability to achieve thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool
5. Examines the impact of process variables on melt pool depth and trailing edge length for the range of process variables likely to produce equiaxed grain growth at the deepest point in the melt pool

7.2 Summary

In order to fully realize the potential of additive manufacturing, it is necessary to achieve consistent and desirable microstructure. While columnar grain morphology may be obtained for additive manufacturing of Ti-6Al-4V, purely equiaxed grain morphology has not been obtained through process parameter controls. Prior work has determined that equiaxed grains are attainable at the surface of the melt pool and has presented a methodology by which process variables may be related to predicted grain morphology. Using a variation on this methodology, this work examines the response of thermal conditions at the deepest point in the melt pool to predict the combination of process variables necessary to obtain a purely equiaxed grain morphology. The results are strictly applicable for the case of a melt pool on a semi-infinite substrate with no added material, with the observation that obtaining thermal conditions favorable for equiaxed grain growth at the deepest point in the melt pool is equivalent to obtaining thermal conditions favorable for equiaxed grain growth through the entirety of the melt pool.

This work predicts that thermal conditions favorable for equiaxed grain growth cannot be obtained for the 25°C (no preheat) case by changing beam power and velocity. Introducing a process preheat decreases the thermal gradient at solidification. If a high enough preheat is selected (~75-90% of liquidus temperature) together with an appropriate power-velocity combination, conditions favorable for equiaxed grain growth can theoretically be obtained at the deepest point in the melt pool.

Consideration of four representative commercial processes suggests that existing processes lack the preheat capabilities necessary to achieve fully equiaxed morphology through process variable control. Of the four processes considered—LENS, Sciaky, EOS,
and Arcam—Sciaky would be the best process to modify with an increased preheat because of its high power beams and comparatively low velocities. However, for substrate preheat temperatures at or above 89% of the liquidus temperature (1475°C), a modified LENS process would work just as well, if not better.

Due to the trends in melt pool size observed for the processes, a process capable of producing equiaxed grain growth at the deepest point in the melt pool is expected to be on the centimeter scale. However, examination of melt pool size, specifically melt pool depth and trailing edge length, for the range of process variables expected to produce equiaxed grain growth at the deepest point in the melt pool suggest that absorbed power and velocity directly impact melt pool geometry. Substrate preheat temperature only meaningfully impacts melt pool geometry by restricting the range of powers and velocities expected to produce equiaxed grain growth at the deepest point in the melt pool. This means that the substrate will not turn into a giant melt pool in response to preheat temperatures as high as 94% of the liquidus melt temperature (1550°C)! Indeed, using this high of a substrate preheat allows for the use of a low power source resulting in a very small melt pool. For the case of a 100 W absorbed power traveling at 100 mm/s using this preheat, the melt pool is expected to be less than 1 mm deep and about 0.25 cm in length.

7.3 Conclusions

Thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool:

- Are theoretically possible to obtain
- Require a substrate preheat temperature at least ~75% of the liquidus temperature
- Do not necessarily correspond to a very large melt pool
  - Melt pool trailing edge length depends primarily on absorbed power.
  - Melt pool depth is a function of power and velocity.
  - Substrate preheat limits the range of powers and velocities that are likely to produce thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool.
- Cannot be obtained through process variable control by the four commercial processes considered: LENS, Sciaky, EOS or Arcam
  - Both LENS and Sciaky operate in the necessary range of powers and velocities. However, they lack the necessary preheat
    - Select which one, either LENS or Sciaky, to modify by adding preheat based on the size of the melt pool needed for a given application.
  - EOS and Arcam operate at a higher velocity range at which obtaining equiaxed morphology is more difficult. Additionally, they lack the necessary preheat.
Summary of Conclusions:

- Thermal conditions favorable to equiaxed grain growth cannot be obtained at the deepest point in the melt pool through process variable control without the introduction of a near-melt-temperature preheat.
- If adding a near-melt-temperature preheat is not feasible for a given process or application, an alternative method for obtaining equiaxed morphology is necessary.

7.4 Future Work

The entirety of this work utilizes a modification of Bontha’s analytical model. This model, using the 3-D Rosenthal solution, ignores latent heat effects and assumes that material properties are independent of temperature. Sources in published literature confirm that this approach provides an accurate qualitative description of behavioral trends at solidification [3, 14-16]. In order to provide quantitatively accurate information, it is necessary to conduct finite element modeling in order to take into account latent heat and the temperature dependence of material properties. Experimental testing should be conducted to confirm morphology predictions, particularly at the power-velocity-preheat combinations projected to yield equiaxed grain growth at the deepest point in the melt pool.

From a manufacturing standpoint, the adaptability of existing processes needs to be considered as well as the variety of ways in which a near-melt-temperature preheat condition could be applied. In terms of materials and microstructure, it is important to determine the impact of keeping the entire build above the beta transus temperature. This work gives no consideration to the alpha laths expected to form within the prior beta grains. Similarly, no attention is given to the impact of added material. The assumption that thermal conditions favorable to equiaxed grain growth at the deepest point in the melt pool are equivalent to such conditions throughout the melt pool depth should be carefully considered in this context.

Very little has been done in terms of exploring process space for near-melt-temperature substrate preheat conditions. No equations currently exist to describe the families of curves presented in Section 6.4.2: Investigation of Melt Pool Size for Near-Melt-Temperature. Consideration should be given to preheat temperatures above and below those considered here as well, particularly once the addition of latent heat effects and the temperature dependence of properties can be taken into account and the exact process space boundaries of the equiaxed morphology region determined. Of particular interest is the asymptotic boundary behavior seen for minimum thermal gradient vs. maximum solidification rate at the deepest point in the melt pool for a given preheat temperature. Additional analytical models may build on the work begun in the Appendices.

Exploratory work, provided in Appendix B, suggests that dimensionless relationships exist relating solidification rate and thermal gradient at the deepest point in the melt pool
to the corresponding values at the surface of the melt pool. Further examination of these relationships is warranted, as in situ monitoring is only possible for the top surface of the melt pool. If information about thermal conditions at the deepest point in the melt pool is obtainable as a function of the same conditions at the surface, then knowledge obtained through in situ monitoring can be used to determine thermal conditions throughout the depth of the melt pool.

Additional literature review and exploratory work concerning Hunt’s criterion boundary curves are provided in Appendix A. By manipulation of Hunt’s original equations, a direct relationship between thermal gradient and solidification rate is obtainable as a function of material properties and a single, experimentally determined constant. If these values can be obtained, then characterization of process behavior across alloy systems will be greatly simplified, as process characterization for certain alloys of interest is seriously impeded by the absence of published Hunt’s criterion boundary curves for those alloys.
Appendices

Appendix A : Hunt’s Curves
A-1 Original Hunt’s Criterion Curves
A-2 Adaptation of Hunt’s Criterion for Additively Manufactured Ti-6Al-4V

Appendix B : Rosenthal Curve Fit Relationships
B-1 Rosenthal Curve Fit Relationships
B-2 Calculation of Coefficient of Determination, \( r^2 \)

Appendix C : Sample MATLAB Code
C-1 MATLAB Code for Plotting Hunt’s Criterion Curves
C-2 MATLAB Code for 3-D Rosenthal Solution
C-3 MATLAB Code Used to Plot Solidification Maps
Appendix A: Hunt’s Curves

A-1 Original Hunt’s Criterion Curves

Hunt’s criterion boundary curves divide the range of possible thermal gradients and solidification rates into three regions: the range of thermal conditions favorable to columnar grain growth, the range of conditions favorable to equiaxed grain growth, and the intermediate region where a mixed morphology is likely to form [5].

For this analysis, Hunt considers what he refers to as “the steady state equiaxed growth problem.” Critical assumptions include:

1) Time independence: For each temperature, the number and size of the equiaxed grains, taken over a large enough area, remain constant with respect to time.
2) One-dimensionality: Temperature does not change in the plane perpendicular to the x-direction (direction of grain growth).
3) No appreciable motion during formation: Equiaxed crystals do not move applicably before they either impinge or are overtaken by the columnar growth front.
4) Heterogeneous nucleation: Equiaxed grains are formed by heterogeneous nucleation.
5) Simultaneous nucleation: All nucleation sites available operate as soon as the heterogeneous nucleation temperature is reached.
6) Negligible heat evolved: The temperature gradient is not appreciably affected by the heat evolved during grain growth.
7) Low velocity limitation: High thermal gradient and very low velocity do not occur in conjunction. That is,

\[ \frac{GD}{V} \ll A'(C_0R)^{1/2} \]  \hspace{1cm} A-1.1

where \( G \) is the thermal gradient, \( D \) is the liquid diffusion coefficient, \( C_0 \) is the alloy composition, \( R \) is the velocity of the solidification front and \( A' \) is a constant. [5]

8) Morphology definition: Fully equiaxed growth corresponds to \( \phi \) greater than 0.49, where \( \phi \) is defined to be the volume fraction of equiaxed crystals present when the columnar front passes. Fully columnar growth has a volume fraction around 1% of this value. That is,

\[ \varphi_{\text{equiaxed}} \geq 0.49 \]
\[ \varphi_{\text{columnar}} \leq 0.01\varphi_{\text{equiaxed}} \Rightarrow \varphi_{\text{columnar}} \leq 0.0049 \]  \hspace{1cm} A-1.2
Pursuant to these assumptions and through consideration of equiaxed grain growth during directional solidification, Hunt derived the following inequalities:

\[
G < 0.617 N_0^{1/3} \left( 1 - \frac{(\Delta T_N)^3}{(\Delta T_c)^3} \right) \Delta T_c \quad \text{Fully Equiaxed Growth} \quad A-1.3
\]

\[
G > 0.617(100N_0)^{1/3} \left( 1 - \frac{(\Delta T_N)^3}{(\Delta T_c)^3} \right) \Delta T_c \quad \text{Fully Columnar Growth} \quad A-1.4
\]

where \( G \) is the thermal gradient, \( N_O \) is the total number of heterogeneous substrate particles originally available per unit volume, and \( \Delta T_N \) is the undercooling at the heterogeneous nucleation temperature [5]. The undercooling \( \Delta T_c \) is equal to that of the columnar growth front temperature

\[
\Delta T_c = \left( \frac{R C_o}{A} \right)^{1/2} \quad A-1.5
\]

where \( A \) is a constant and \( R \) and \( C_o \) are the same as for Equation A-1.1 [5].

Substituting Equation A-1.5 into Hunt’s inequalities (Equations A-1.3 & A-1.4) provides a direct relationship between thermal gradient and solidification rate:

\[
G(R) < 0.617 N_0^{1/3} \left( 1 - (\Delta T_N)^3 \left( \frac{R C_o}{A} \right)^{-3/2} \right) \left( \frac{R C_o}{A} \right)^{1/2} \quad \text{Equiaxed} \quad A-1.6
\]

\[
G(R) > 0.617(100N_0)^{1/3} \left( 1 - (\Delta T_N)^3 \left( \frac{R C_o}{A} \right)^{-3/2} \right) \left( \frac{R C_o}{A} \right)^{1/2} \quad \text{Columnar} \quad A-1.7
\]

Hunt’s values of \( N_O \), \( \Delta T_N \), \( C_o \), and \( A \) for Al-3wt.%Cu are summarized below in Table A-1-1. Note that this implies units of K/mm for \( G \) and \( \mu m/s \) for \( R \).

**Table A-1-1: Summary of Hunt’s Equation Parameters (Al-3wt.%Cu)**

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Units</th>
<th>Al-3wt.%Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_O )</td>
<td>mm(^3)</td>
<td>1</td>
</tr>
<tr>
<td>( A )</td>
<td>( \mu m \ s^{-1} ) (wt.%)(^{-1}) K(^{-2})</td>
<td>300</td>
</tr>
<tr>
<td>( \Delta T_N )</td>
<td>K</td>
<td>0.75</td>
</tr>
<tr>
<td>( C_o )</td>
<td>(wt.%)(^{-1})</td>
<td>3</td>
</tr>
</tbody>
</table>
A-2 Adaptation of Hunt’s Criterion for Additively Manufactured Ti-6Al-4V

In 2003, Kobryn and Semiatin experimentally considered the relationship between solidification rate, thermal gradient at solidification, and grain morphology for Ti-6Al-4V castings and laser glazes [6]. As stated in [6], a clear boundary was observed between the equiaxed, columnar and mixed morphology regions. Thus, Hunt’s curves were scaled and added to a plot of thermal gradient versus solidification rate. By implication, the applicability of the scaled Hunt’s curves is not directly limited by the assumptions governing its derivation. That is, Hunt’s criterion curves can be applied to experimental data formed by processes not governed by the assumptions listed in the previous section. Previous researchers have applied a version of Hunt’s criterion curves to additive manufacturing for Inconel and titanium with favorable results [3, 10-12, 18].

For this work, it is not necessary to determine an improved version of Hunt’s curves for Ti-6Al-4V. Rather, for ease of plotting, an equation in G and R is desired for each of the two boundary curves. From an internal report, the data points summarized in Table A-2-1 were employed by Kobryn to obtain the scaled Hunt’s curves seen in [6].

Table A-2-1: Hunt’s Curve Translation to Ti-6Al-4V Curve Fit Points

<table>
<thead>
<tr>
<th>R (cm/s)</th>
<th>G (K/cm)</th>
<th>Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0045</td>
<td>10.6</td>
<td>Columnar</td>
</tr>
<tr>
<td>0.0047</td>
<td>40.2</td>
<td>Columnar</td>
</tr>
<tr>
<td>0.005</td>
<td>81.3</td>
<td>Columnar</td>
</tr>
<tr>
<td>0.01</td>
<td>489</td>
<td>Columnar</td>
</tr>
<tr>
<td>0.1</td>
<td>2170</td>
<td>Columnar</td>
</tr>
<tr>
<td>1</td>
<td>6940</td>
<td>Equiaxed</td>
</tr>
<tr>
<td>10</td>
<td>22000</td>
<td>Equiaxed</td>
</tr>
<tr>
<td>100</td>
<td>69400</td>
<td>Equiaxed</td>
</tr>
<tr>
<td>1000</td>
<td>220000</td>
<td>Equiaxed</td>
</tr>
</tbody>
</table>

Given Hunt’s curves in terms of $G$ and $R$, as in Equations A-1.6 and A-1.7, smooth curves that pass through the points provided by Kobryn can be obtained by changing the material-dependent constants $C_O$, $N_O$, $\Delta T_N$ and $A$. First, the composition, $C_O$, is approximated as the total weight percent of non-titanium (non-base metal) present in the alloy. Utilizing the alloy composition from [45], $C_O$ is approximated to be 12.27 (wt %)$^{-1}$. Various values of $N_O$, $\Delta T_N$ and $A$ were plotted, as shown below in Figure A-2-1.
Based on observation of the general impact of changing $N_O$, $\Delta T_N$, and $A$, these three values were iteratively adjusted until the resultant equations passed through the center of the points provided in Table A-2-1. Using this methodology, values of $C_O$, $N_O$, $\Delta T_N$ and $A$ were selected to form smooth curves. Figure A-2-2(a) displays the curves formed from these values, while Figure A-2-2(b) shows a set of previously published Hunt’s curves for Ti-6Al-4V. The circles in Figure A-2-2(a) correspond to the points from Table A-2-1.  

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12 See Appendix C-1 for MATLAB code concerning Hunt’s Curves
Figure A-2-2: Hunt’s Curves in Ti-6Al-4V

(a) Re-Created Hunt’s Curves

(b) Previously published [15]
Appendix B: Rosenthal Curve Fit Relationships

B-1 Rosenthal Curve Fit Relationships

When viewing the accumulated Rosenthal data from nearly two hundred process variable combinations, several interesting trends emerged. Three of these trends feature dimensionless relationships between process variables and outcomes.

The first of the dimensionless relationships is that observed between the natural logarithm of the nondimensionalized liquidus temperature, \( \overline{T}_m \), and dimensionless melt pool depth, \( \overline{d} \). Initial observation suggested an exponential relationship. The initial, exponential curve fit equation, shown below as Equation B-1.8, had a coefficient of determination of \( r^2 = 0.8897 \).

\[
\overline{d} = e^{-0.44 \ln(\overline{T}_m)} \tag{B-1.8}
\]

Using an iterative methodology to improve the curve fit yields the equation provided in Equation B-1.9, which has a coefficient of determination of \( r^2 = 0.9976 \):

\[
\overline{d} = 4.5 \times 10^{-3} (\overline{T}_m - 4)^3 + e^{-0.4676 \ln(\overline{T}_m)} \tag{B-1.9}
\]

Both curve fit equations are plotted together with the Rosenthal data below in Figure B-1-1.

---

13 Equations used to determine coefficient of determination, \( r^2 \), are provided in Appendix B-2
The next two dimensionless relationships are of particular interest as they concern thermal conditions at the depth of the melt pool, the thermal gradient and solidification rate. Unlike dimensionless depth, the thermal gradient and solidification rate at melt pool depth are not directly related to the natural logarithm of nondimensionalized temperature but are considered as dimensionless ratios. These ratios are presented in Equation B-1.10 as:

\[ G_{ratio} = \frac{g_{depth}}{g_{surf}} \text{ and } R_{ratio} = \frac{R_{depth}}{R_{surf}} \]  

Initial observation suggests an exponential relationship between the thermal gradient ratio and the natural logarithm of nondimensionalized temperature, \( \bar{T}_m \). As for dimensionless depth, an initial, exponential curve fit is applied. This exponential curve fit, provided below as Equation B-1.11, had a coefficient of determination of \( r^2 = 0.8928 \):

\[ G_{ratio} = e^{-0.5 \ln(\bar{T}_m)} \]
Using the same iterative methodology to improve the curve fit yields the equation provided below in Equation B-1.12, which has a coefficient of determination of $r^2 = 0.9981$:

$$G_{ratio} = 1.78 \cdot e^{-0.47 \ln(T_m)} + 0.0046(T_m - 3.5)^3 + 0.034(T_m - 3.5)^2 + 0.3T_m - 1$$  \hspace{1cm} B-1.12

Both curve fit equations are plotted together with the Rosenthal data below in Figure B-1-2.

![Figure B-1-2: Relationship between Thermal Gradient Ratio and Dimensionless Temperature](image)

The relationship between solidification rate ratio and the natural logarithm of nondimensionalized temperature, $T_m$, is more complex. Initial observation suggests an inverse tangent relationship. An initial curve fit is applied and its equation provided below in Equation B-1.13 as

$$R_{ratio} = \frac{1}{3\pi} \tan^{-1}(8 \ln(T_m) + 1) + 0.125$$  \hspace{1cm} B-1.13

While describing the general shape of the curve, this curve fit cannot be utilized to predict solidification rate based on dimensionless temperature and beam velocity, as seen in Figure B-1-3. The iteratively improved curve fit, provided in Equation B-1.14, provides a much better description of the relationship. The coefficient of determination for Equation B-1.14 is $r^2 = 0.9953$, as compared to Equation B-1.13, with a coefficient of determination of $r^2 = 0.3391$. 

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\[ R_{ratio} = real\left(0.1217 + 0.0732 \times \tan^{-1}\left(\frac{37x + 80}{72}\right) + 0.007516x^{1/2} - 0.02122x^{1/3}\right) \]

\[ x = \ln\left(\frac{T_m}{Tmbar}\right) \]

Both curve fit equations are plotted together with the Rosenthal data below in Figure B-1-3.

**Figure B-1-3: Relationship between Solidification Rate Ratio and Dimensionless Temperature**

Combined, Figure B-1-2 and Figure B-1-3 provide a means of calculating thermal gradient and solidification rate at the deepest point in the melt pool based on the corresponding values at the top surface. Since the thermal gradient and solidification rate at the deepest point in the melt pool determine whether or not fully equiaxed grain growth is expected to occur, these dimensionless relationships provide a mechanism by which solidification microstructure at melt pool depth may be calculated in terms of process variables (\(\overline{T_m}\)) and thermal conditions at the top surface of the melt pool, which may ultimately be linked to direct observation of melt pool geometry based on in-situ process monitoring.
**B-2 Calculation of Coefficient of Determination, \( r^2 \)**

The coefficient of determination, \( r^2 \), is determined according to [46, 47] as:

\[
SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\
SST = \sum_{i=1}^{n} (y_i - \bar{y})^2 \\
r^2 = 1 - \frac{SSE}{SST}
\]

where \( y_i \) represents each of the data values, \( \hat{y}_i \) is the curve fit value corresponding to data point \( y_i \) and \( \bar{y} \) is the mean of the data.
Appendix C: Sample MATLAB Code

C-1 MATLAB Code for Plotting Hunt’s Criterion Curves

C-1.1 Iteration Toward Finalized Parameters:

```matlab
% % HuntsCurveRecreation_Ti64.m
% % Sarah Kuntz, 2015
close all
clear all
clc

%% Re-creating Hunt's Curves for Ti64
fig2save= figure;
figpath=’C:\Users\Sarah\Desktop\RA--Research files\My_Attempt\Hunts_Trends\’;

R_val = [0.00001:0.00001:0.00045, 0.00001:0.00045:.0001:0.01-.0001, 0.01:1-.01, 1:10:1000]; % cm/s Vector of Solidification Rates
colorstr=[’k’,’b’,’g’,’r’,’c’,’m’,’y’];
% Properties changed for this system:
No=7; % l/mm^3
A_vect=[0.01,0.1,1,10,100,500,1000]; % 750 um/(s*wt%*K^2)
Co=12.27; % Ti 64
delta_TN=0.85; % K

for i=1:length(A_vect)
A=A_vect(i);
delta_Tc=(10000*R_val.*Co/A).^(1/2); % K
G_eq = 0.617*(No^(1/3)*10).*(1-(delta_TN.^3)./(delta_Tc.^3)).*delta_Tc;
% G_col = 0.617*((100*No)^(1/3)*10).*(1-
  (delta_TN.^3)./(delta_Tc.^3))...
  .*delta_Tc;
% Plot Hunt's Criterion Curves for Ti-6Al-4V:
loglog(R_val,G_eq*10,colorstr(i))
% loglog(R_val,G_col*10,R_val,G_eq*10)
hold on
end

for i=1:length(A_vect)
A=A_vect(i);
delta_Tc=(10000*R_val.*Co/A).^(1/2); % K
G_eq = 0.617*(No^(1/3)*10).*(1-(delta_TN.^3)./(delta_Tc.^3)).*delta_Tc;
G_col = 0.617*((100*No)^(1/3)*10).*(1-(delta_TN.^3)./(delta_Tc.^3))...
  .*delta_Tc;
% Plot Hunt's Criterion Curves for Ti-6Al-4V:
loglog(R_val,G_col*10,[’:’,colorstr(i)])
% loglog(R_val,G_col*10,R_val,G_eq*10)
hold on
end
```

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% Plot Hunt's Criterion Curves for Ti-6Al-4V:
loglog(R_val,G_eq*10,colorstr(i),'LineWidth',2)
% loglog(R_val,G_col*10,R_val,G_eq*10)
hold on
exlabel('Solidification Rate, R (cm/s)','FontSize',14);
ylabel('Thermal Gradient, G (K/cm)','FontSize',14)
plot_title='Hunts_Curves_Changing_A';
title('Hunt's Curves: Changing A','FontSize',16);
legend(['A = ',num2str(A_vect(1))],['A = ',num2str(A_vect(2))],...
     ['A = ',num2str(A_vect(3))],['A = ',num2str(A_vect(4))],...
     ['A = ',num2str(A_vect(5))],['A = ',num2str(A_vect(6))],...
     ['A = ',num2str(A_vect(7))],'location','SouthEast')

% saveas(fig2save,[figpath,plot_title,'.jpg'])%Save
xlim([1e-4 1e3])
ylim([1e-2 1e6])

Figure C-1-1: Expected Output from MATLAB Code in Section C-1.1

C-1.2 Smoothly Plots Hunt's Curves
% Set Up Figure Window
fig1=figure; set(fig1,'Position',[403 49 789 635]);
% Plot Hunt's Curves
R_val = [0.00045:.0001:0.01,.01:0.1:1-0.1,1:10:1000]; % cm/s
G_eq=1509.650.*R_val.^(1/2).*(1-2.9348e-4.*R_val.^(3/2));
G_col=7006.9.*R_val.^(1/2).*(1 - 2.9348e-04.*R_val.^(3/2));
loglog(R_val,G_col,'--k',R_val,G_eq,'k','LineWidth',2);
hold on
% Set Up Axes
xlim([1e-4 1e3]); ylim([1e0 1e6])
set(gca,'linewidth',2,'FontSize',12,'FontWeight','bold');
x_label=[1e-4,1e-3,1e-2,1e-1,1e1,1e2,1e3];
y_lab=[1,1e1,1e2,1e3,1e4,1e5,1e6];
set(gca,'XTick',x_lab,'YTick',y_lab);
axis square
% Add Morphology Labels
text(2e-4,5e5,'Columnar Grains','FontSize',12,'Color',[0 0 0],...
    'FontAngle','italic','FontWeight','bold')
text(1e1,7e2,'Equiaxed Grains','FontSize',12,'Color',[0 0 0],...
    'FontAngle','italic','FontWeight','bold')
text(1e-1,1e3,'Mixed Morphology','FontSize',12,'Color',[0 0 0],...
    'FontAngle','italic','Rotation',30,'FontWeight','bold')
% Put Mixed Label at center (1e-1,1e3); far right (1e1,1.25e4)
% Axis Labels & Title
xlabel('Solidification Rate (cm/s)','FontSize',14,'FontWeight','bold')
ylabel('Thermal Gradient (K/cm)','FontSize',14,'FontWeight','bold')
title('Hunt''s Curves for Ti-6Al-4V','FontSize',16,'FontWeight','bold')

Figure C-1-2: Expected Output from MATLAB Code in Section C-1.2
C-2 MATLAB Code for 3-D Rosenthal Solution

C-2.1 Script Files Called by Rosenthal Iterator

C.2.1.1 Function file: f3d.m

```matlab
function value = f3d(x0bar, Tmbar, z0bar)
% Subtracts dimensionless Rosenthal temperature T(x0bar, z0bar) from
% dimensionless temperature Tmbar. Where value equals zero, x0bar and
% z0bar lie on the Tmbar isotherm.
% *Note: y0bar is not included because y0bar = 0 (along center of melt
% pool)
value = Tmbar - 0.5*(((exp(-(x0bar + sqrt(x0bar^2 + ...
    z0bar^2))))/(sqrt(x0bar^2 + z0bar^2))));
end
```

C.2.1.2 Function file: NDLookUp.m

```matlab
function [ L, ND ] = NDLookUp( Tmbar )
% Given dimensionless temperature Tmbar (found using the liquidus
% temperature):
% 1) Calculate x0-direction initial guess, L, from Sheridan's
% Relationship: L = -1./(2*TmLbar);
% 2) Select z0-direction initial guess, ND, from Kuntz's look-up
% table.
% *Note: ND values may need adjustment close to bin boundaries
L=-1/(2*Tmbar);

if Tmbar < 4.39e-6; ND=600;
elseif Tmbar < 1e-5; ND=300;
elseif Tmbar < 4e-5; ND=200;
elseif Tmbar < 0.00015; ND=100;
elseif Tmbar < 0.0005; ND=50;
elseif Tmbar < 0.001; ND=30;
elseif Tmbar < 0.0025; ND=20;
elseif Tmbar < 0.005; ND=13;
elseif Tmbar < 0.015; ND=10;
elseif Tmbar < 0.03; ND=5;
elseif Tmbar < 0.05; ND=5;
elseif Tmbar < 0.1; ND=3.4;
elseif Tmbar < 0.2; ND=2.2;
elseif Tmbar < 0.25; ND=1.75;
elseif Tmbar > 0.25; ND=0.7713*Tmbar^-0.528;
end
end
```
C.2.1.3 Function file: NTG_Ros3D.m

```matlab
function [ NTG ] = NTG_Ros3D(X,Z)
% Uses 3D Rosenthal solution to find nondimensional thermal gradient
% at relative coordinate (X,0,Z)
sum_xyz = X^2+Z^2; % Y^2=0
sqrt_xyz = sqrt(sum_xyz); % sqrt(X^2+Y^2+Z^2), Y^2=0
ThermX = -1/2*exp(-(X-sqrt_xyz))/sqrt_xyz*(1+X/sqrt_xyz+X/sum_xyz); % ThermY_loop1(m) = 0
ThermZ = -1/2*Z*exp(-(X-sqrt_xyz))/sum_xyz*(1+1/sqrt_xyz);
NTG = sqrt(ThermX^2+ThermZ^2);
end
```

C.2.2 Rosenthal_Iterator.m

```matlab
%% Rosenthal_Iterator
% Determines properties at 99% of Melt Pool Depth & saves values in Excel spreadsheet
% Can enter power, velocity & Preheat temperature as vectors.
clear all
close all
clc

% *NOTE: THESE FILES MUST BE SAVED IN THE SAME DIRECTORY AS THIS FILE:
% f3d.m                 % Purpose: Function file used for root finding
% NTG_Ros3D.m           % Purpose: Determine dimensionless thermal gradient
% NDLookUp.m            % Purpose: Use Tmbar to determine initial guesses for root finding

% EXTERNAL FUNCTIONS REQUIRED

% VARIABLE INPUTS

TableName='LENS_test_case_1.xlsx'; % Excel spreadsheet name
aPower=[100,500,1000,10000]; % Absorbed power (Watts)
Velocity=[4.23,635]; % Velocity (mm/s)
preheat=[25,750]; % Preheat temperature (deg C)
num_of_pts=5000; % Number of points for iteration through depth
precision = 0.99; % Percentage of depth at which to find properties at (99% of depth)

% MATERIAL PROPERTIES for Ti-6Al-4V

TmL = 1654; % deg C, Liquidus Temperature
TmS = 1620; % deg C, Solidus Temperature
rho = 4002.22782; % Mass Density (kg/m^3) at Liquidus
c = 857.6789; % Specific Heat (J/(kg deg C)) at Liquidus
k = 30.454; % Thermal Conductivity (W/(m*K)) at Liquidus

% USER DEFINED FUNCTIONS

% Dimensionalizes thermal gradient (K/cm)
G_DIMcm = @(val,aQ,v) ((rho*c*v)/(2*k))^2*(aQ/(pi*k)).*val./100;
% Dimensionalizes cooling rate (K/s)
CR_DIMs = @(val,aQ,v) ((rho*c*v)/(2*k))^2*((aQ*v)/(pi*k)).*val;
% Dimensionalizes position/spatial coordinates (cm)
```

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\[ xz_{\text{DIMcm}} = @(\text{val},v) \text{(val).} \ast (2\ast k)/(\rho \ast c \ast v) \ast 100; \]

\[ \text{FIND\_NCR3D} = @(X,Z) 0.5 \ast \text{exp}(-\left(\begin{array}{c} X + \sqrt{X^2+Z^2} \end{array}\right))/\sqrt{X^2+Z^2}\ldots \ast (1 + X/\sqrt{X^2+Z^2} + X/(X^2+Z^2)); \]

\% Finds 3-D nondimensional cooling rate for relative coordinate
\% (X,0,Z):
\% FIND\_NCR3D = @(X,Z) 0.5*exp(-X + sqrt(X^2+Z^2))/sqrt(X^2+Z^2)...
\%*(1 + X/sqrt(X^2+Z^2) + X/(X^2+Z^2));

\% %----------------------------- ITERATIVE LOOPS ----------------------------- %
row=0; \% Specify initial value; 'row' corresponds to the row in the
\% spreadsheet to which the data will be saved
for I=1:length(preheat) \% For each Preheat temperature
T0=preheat(I); \% Rename the Preheat for this iteration 'T0'
for j=1:length(aPower) \% For each power
aQ=aPower(j); \% Rename the power for this iteration 'aQ'
for i=1:length(Velocity) \% For each velocity
v=Velocity(i)./1000; \% Convert velocity for this iteration
to m/s & rename 'v'
row=row+1; \% Increase counter
\%
\% Nondimensionalize Liquidus & Solidus Temperatures
TmLbar = ((TmL - T0)/((aQ/(pi*k))\ast((\rho\ast c\ast v)/(2\ast k))));
TmSbar = ((TmS - T0)/((aQ/(pi*k))\ast((\rho\ast c\ast v)/(2\ast k))));
\%
\% Determine initial guesses for root finding; L is x-dir,
\% ND is z-dir guess
[L,ND] = NDLookUp(TmLbar); \% NDLookUp is an external
\% function file
x0barL(1)=L; \% Set the first entry in the liquidus x0bar
\% vector to the initial guess
x0barS(1)=L; \% Use the same initial guess for the solidus
\% x0bar vector
\%
\% Finding Isotherms & finding thermal conditions there
\% ________________ FIRST ITERATIVE LOOP ________________
\% Purpose of this loop: Improve initial guesses ND & L
\% m=1; \% Initial value for counter
\% D = linspace(0,ND,num_of_pts)'; \% Vector of incremental
\% depths
while m <= num_of_pts \% Do the following until...
\% Store m-th incremental depth in z0bar
\% Use external function f3d to find x0:
\[ xL(m), \sim, \text{EXITFLAGL} \] = fzero(@f3d,x0barL(m), [], ... 
\[ \text{TmLbar, z0bar(m)); \% liquidus isotherm} \]
\[ xS(m), \sim, \text{EXITFLASG} \] = fzero(@f3d,x0barS(m), [], ... 
\[ \text{TmSbar, z0bar(m)); \% solidus isotherm} \]
\% if EXITFLAGL < 1 \% If liquidus isotherm doesn't exist
\% at this incremental depth:
\% Set ND equal to the last OK depth z0bar(m-1) &
\% add 1 increment, so ND will be larger than
\% expected depth.
\% Thus: ND_new=z0bar(m-1)+delta=z0bar(m)
ND= z0bar(m); \% 'corrected' ND
\% if ND == 0 \% If ND=z0bar=0 (aka top of melt pool),
% then initial ND guess was probably too big. % User must correct this error. Display:
fprintf(2,['
!!! ERROR: ND ESTIMATE TOO ',...  
'LARGE!! Error in Rosenthal_Iterator.m',...  
' FIRST ITERATIVE LOOP !!! 
']);
break % Exit loop

break % Exit loop / stop increasing depth
elseif EXITFLAGS < 1 % Just in case:
fprintf(2,['
!!! ERROR: PROBLEM WITH SOLIDUS',...  
'ISOTHERM!!! Error in Rosenthal_Iterator.m',...  
'FIRST ITERATIVE LOOP !!! 
']);
break % Exit loop

x0barL(m+1) = xL(m); x0barS(m+1) = xS(m); % Store % values
m=m+1; % Increase counter
end

%% ----------------- SECOND ITERATIVE LOOP -----------------
fixed_x0bar_guessL = x0barL(2); % "Store" corrected x0 % guesses
fixed_x0bar_guessS = x0barS(2);
clear D EXITFLAGL EXITFLAGS m MeltpoolDepth xL xS ...
 x0barL x0barS z0bar D

% Apply corrected x0 guesses for root finding
x0barL(1) = fixed_x0bar_guessL;
x0barS(1) = fixed_x0bar_guessS;
D = linspace(0,ND,num_of_pts); % Incremental depth vector
m = 1; % Re-set counter

while m <= num_of_pts % Do the following until...
z0bar(m)=D(m); % Store incremental depth in z0bar % vector
% Use external function f3d to find x0:
[xL(m),~,EXITFLAGL] = fzero(@f3d,x0barL(m),[],...  
TmLbar,z0bar(m)); % on the liquidus isotherm
[xS(m),~,EXITFLAGS] = fzero(@f3d,x0barS(m),[],...  
TmSbar,z0bar(m)); % on the solidus isotherm

if EXITFLAGL < 1 % See explanation from FIRST ITERATIVE % LOOP
  ND=z0bar(m);
  if ND == 0
    fprintf(2,['
!!! ERROR: ND ESTIMATE TOO ',...,  
'LARGE!! Error in Rosenthal_Iterator.m',...,  
' SECOND ITERATIVE LOOP !!! 
']);
  end
  break
elseif EXITFLAGS < 1
  fprintf(2,['
!!! ERROR: PROBLEM WITH SOLIDUS',...,  
'ISOTHERM!!! Error in Rosenthal_Iterator.m',...  
'SECOND ITERATIVE LOOP !!! 
']);
}
break
end

% Find Dimensionless, Instantaneous Cooling Rate & % Dimensionless Thermal Gradient at solidus & liquidus % isotherms for each x0-z0 coordinate pair:
NCR_L(m) = FIND_NCR3D(xL(m),z0bar(m));
NCR_S(m) = FIND_NCR3D(xS(m),z0bar(m));
NTGL(m) = NTG_Ros3D(xL(m),z0bar(m));
NTGS(m) = NTG_Ros3D(xS(m),z0bar(m));
x0barL(m+1) = xL(m); x0barS(m+1) = xS(m); % Store % values
m=m+1; % Increase counter
end

% ---------------- COLLECT & DIMENSIONALIZE RESULTS ----------------

% Length of vectors multiplied by precision --> index of % depth
Length_of_Loop2=m-1; iod=round(precision*Length_of_Loop2);
dimensionless_depth=z0bar(iod); % Dimensionless depth (for % reference)

% Results at Surface / Top of Melt Pool
% Thermal Gradient at surface (K/cm)
GLsurf = G_DIMcm(NTGL(1),aQ,v);
GSsurf = G_DIMcm(NTGS(1),aQ,v);
% Instantaneous Cooling Rate (K/s) at surface [liquidus]
CRLsurf = CR_DIMs(NCR_L(1),aQ,v);
% x0-coordinate of isotherms at surface (cm)
xL_surf_cm = xz_DIMcm(xL(1),v);
xS_surf_cm = xz_DIMcm(xS(1),v);
% z0 at surface (cm) [should be zero]
z_surf_cm = xz_DIMcm(z0bar(1),v);

% Results at Depth / Bottom of Melt Pool
% Thermal Gradient at depth (K/cm)
GL = G_DIMcm(NTGL(iod),aQ,v); GS = G_DIMcm(NTGS(iod),aQ,v);
% Instantaneous Cooling Rate (K/s) at depth, for sanity % check
CRL = CR_DIMs(NCR_L(iod),aQ,v);
CRS = CR_DIMs(NCR_S(iod),aQ,v);
xL_depth_cm = xz_DIMcm(xL(iod),v); % x0 at depth (cm), % liquidus
xS_depth_cm = xz_DIMcm(xS(iod),v); % x0 at depth (cm), % solidus
z_depth_cm = xz_DIMcm(dimless_depth,v); % z0 at depth (cm), % liquidus

% Results through depth (as a vector)
% **Useful when running a single Power-Velocity-Preheat % combination**

% Thermal Gradient vector (K/cm)
GLvec = G_DIMcm(NTGL,aQ,v); GSvec = G_DIMcm(NTGS,aQ,v);
% Instantaneous Cooling Rate vector (K/s)
CRLvec = CR_DIMs(NCR_L,aQ,v); CRSvec = CR_DIMs(NCR_S,aQ,v);
xL_depth_cmvec = xz_DIMcm(xL,v); % x0 along liquidus (cm)
xS_depth_cmvec = xz_DIMcm(xS,v); % x0 along solidus (cm)
z_depth_cmvec = xz_DIMcm(z0bar,v); % z0 through depth (cm)

% ---------------- COMPUTE COOLING RATE FEA-STYLE ----------------
% Averaged Cooling Rate at depth
% Approximate time btwn isotherms
% (sec = cm/[mm/s]*[10mm/cm])
t_L=xL_depth_cm/Velociy(i)*10;
t_S=xS_depth_cm/Velociy(i)*10;
CR_at_depth = -(TmL-TmS)./(t_L-t_S); % (dT/dt) [C/s <-> K/s]
G_at_depth=mean([GL GS]); % Approx. G ave of L & S (K/cm)
SR_at_depth= -CR_at_depth/G_at_depth; % SR(cm/s)

% Averaged Cooling Rate at surface
% sec
CRave_at_surf = -(TmL-TmS)./(t_Lsurf-t_Ssurf); % [K/s]
G_at_surf=mean([GLsurf GSsurf]); % (K/cm)
SR_at_surf= -CRave_at_surf/G_at_surf; % (cm/s)

% Sanity Check: Average of 2 values should be between them:
if abs(CRL) > abs(CR_at_depth) % If liuidus CR > average
    fprintf(2,['
!!! ERROR: PHYSICAL IMPOSSIBILITY:','
    'LIQUIDUS COOLING RATE MUST BE SMALLER THAN ','
    'AVERAGE!!! Error in Rosenthal_Iterator.m ','
    'COMPUTE COOLING RATE FEA-STYLE 
']);
else abs(CRLsurf) < abs(CR_at_depth)
    fprintf(2,['
!!! ERROR: PHYSICAL IMPOSSIBILITY: ','
    'COOLING RATE AT SURFACE MUST BE LARGER THAN ','
    'COOLING RATE AT DEPTH!!! Error in Rosenthal_Iterator.m ','
    'COMPUTE COOLING RATE FEA-STYLE 
']);
end

% ------------------- SAVE DATA IN TABLE ----------------
% If no table name specified, MATLAB won't save data
if exist('TableName', 'var')==1
    % LABEL is an array of text to label columns of table
    % TABLE is a vector containing the values for this row
    LABEL={'Absorbed Power (W)', 'Velocity in mm/s',... 
    'Substrate Temp (C)'};
    TABLE=[aQ, v*1000, T0]; % Save Inputs
    LABEL=['Tmbar'];
    TABLE=[TABLE, Tmbar]; % Save Tmbar (Liquidus)
    LABEL=['Dimenssionless Depth', 'Depth (cm)',... 
    'xL at Depth (cm)', 'xL at Surface (cm)'];
    TABLE=[TABLE, dimless_depth, z_depth_cm,... 
    xL_depth_cm, xL_surf_cm]; % Save Melt Pool Geometry
    LABEL=['CR at Depth (K/s)',...
    'SR at depth (cm/s)', 'G at depth (K/cm)'];
    TABLE=[TABLE, CR_at_depth, SR_at_depth, G_at_depth];
    LABEL=['CR at surface (K/s)',...
    'SR at surface (cm/s)', 'G at surface (K/cm)'];
    TABLE=[TABLE, CRave_at_surf, SR_at_surf, G_at_surf];
    LABEL=['RunTime'];
TABLE=[TABLE,datestr(now)];

MAT(row,:)=TABLE; clear TABLE % Store row in table
% matrix
end % Close table-creation loop
end % Close velocity loop
end % Close power loop
end % Close Preheat loop
%
if exist('TableName','var')==1 % If table name specified, save data
    sheet=1; % Specify sheet within Excel
    xlswrite(TableName,LABEL,sheet,'A1'); % Write labels in top row
    xlswrite(TableName,MAT,sheet,'A2'); % Write data table to Excel
end
display('ALL DONE!')
### Table C-2-1: Rosenthal Values for a Range of Power-Velocity-Preheat Conditions

Columns A-H:

<table>
<thead>
<tr>
<th>Absorbed Power (W)</th>
<th>Velocity in mm/s</th>
<th>Substrate Temp (C)</th>
<th>Tmbar</th>
<th>Dimensionless Depth</th>
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C-2.1 MorphologyQuickSort.m

*Note: This is a function file. The only input required is the name of that Excel file to be sorted. This is the name of the file that was created by the Rosenthal Iterator

function [] = MorphologyQuickSort(name)
% % Sorts Data into "Equiaxed", "Mixed", and "Columnar" regions
% Enter Name of Excel File to be sorted.
% MorphologyQuickSort is designed to sort files generated by
% RosenthalIterator.m

if strcmp(name(length(name) - 4:length(name)),'.xlsx') == 1
    % If name ends in .xlsx, do nothing; name is fine
elseif strcmp(name(length(name) - 3:length(name)),'.xls') == 1
    % If name ends in .xlsx, do nothing; name is fine
else
    % If name does not end in ".xlsx"
    name=[name,'.xlsx'];
end

[MAT,LABEL]=xlsread(name); % Read in Excel file to sort
[row, col]=size(MAT); % Note dimensions of data

% Set up Possibilities & Counters
EQUIAXED=[]; ect=1;
MIXED=[]; mct=1;
COLUMNAR=[]; cct=1;
EQBORDER=[]; eqb=1;
COBORDER=[]; cob=1;

for i=1:row % For each Power-Velocity-Preheat case in "name"
    Gi=MAT(i,11); Ri=MAT(i,10);
    % Find Hunt's Boundary thermal gradients for this solidification rate
    G_eq=1509.650.*Ri.^(1/2).*((1-2.9348e-4.*Ri.^(3/2)));
    G_col=7006.9.*Ri.^(1/2).*((1-2.9348e-04.*Ri.^(3/2)));
    % And compare the Rosenthal gradient to Hunt's
    % Store that Power-Velocity-Preheat case in the appropriate matrix
    if Gi < G_eq
        EQUIAXED(ect,:) = MAT(i,:); ect = ect+1;
    elseif Gi < G_col
        MIXED(mct,:) = MAT(i,:); mct = mct+1;
    elseif Gi==G_eq
        EQUIAXED(ect,:) = MAT(i,:); ect = ect+1;
    elseif Gi==G_col
        EQBORDER(eqb,:) = MAT(i,:); eqb = eqb+1;
    elseif Gi>G_col
        COLUMNAR(cct,:) = MAT(i,:); cct = cct+1;
    elseif Gi < G_col
        COBORDER(cob,:) = MAT(i,:); cob = cob+1;
    else
        fprintf(['\nERROR in Line 33: Unexpected G value for ', ...
' P=%dW, V=%3fmm/s, T0=%dC'],MAT(i,1:3));
    end
end
% Write to SORTED Excel file (in current directory)
 sname=['SORTED',name];  % New file name, based on "name"

for whichcase=1:5  % For each of the following cases
    switch whichcase
        case 1
            CT=ect; sheet='EQUIAXED'; var=EQUIAXED;
        case 2
            CT=mct; sheet='MIXED'; var=MIXED;
        case 3
            CT=cct; sheet='COLUMNAR'; var=COLUMNAR;
        case 4
            CT=eqb; sheet='EQBORDER'; var=EQBORDER;
        case 5
            CT=cob; sheet='COBORDER'; var=COBORDER;
    end

    if CT > 1  % If data was saved in the matrix, create a sheet with
                % the morphology name & save the data there
        xlswrite(sname,LABEL(1,1:col),sheet,'A1')  % Labels top of sheet
        xlswrite(sname,var,sheet,'A2')
    end
end

display('SORTED!')  % Display output to command window
end
C-3 MATLAB Code Used to Plot Solidification Maps

C-3.1 Script File Used to Plot Results from Rosenthal Iterator

*Note: The solidification rate at depth and thermal gradient at depth columns from the Excel spreadsheet can easily be selected, copied and pasted between the square brackets to form the RG matrix.

```matlab
%% Pretty Plot: Trends
% Sarah Kuntz, 2016
close all; clear all; clc;

wantlegend=1;

name={
    'Impact of Changing Preheat & Velocity';
    'on Thermal Trends at 99% of Melt Pool Depth'};

%% Required Vectors
% preheat, Velocity
% RG=[SR_vec,G_vec]

Velocity=[0.05,0.5,5,10,50,100,500,1000];  % Velocity (mm/s)
preheat=[25,100,500,850,1000,1500];         % Preheat temperature (C)

RG=[0.000969582 10018.60044
    0.009622306 10646.70792
    0.087119616 15433.81372
    0.158190152 19375.89848
    0.521903401 38838.85849
    0.80219272  54565.29052
    1.927096307 122849.7113
    2.76317834  173974.9408
    0.00980499  9111.175401
    0.009694497 9707.700216
    0.087326812 14217.51461
    0.158829904 17900.02255
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    0.089577206 8489.320643
    0.158281431 10920.34768
    0.48705081  22630.01346
    0.728426679 31981.02141
    0.00115438  2405.330304
    0.011272435 2686.369699
    0.092033215 4569.205612
    0.157759647 6010.1818
    0.450707528 12810.30919
}
```
% % % Colors & Symbols for Plot

% colormat: Number of Rows must equal numel(Velocity)
colormat=[0           0         1.0; % Blue
0.75        0         0.75; % Purple / Violet
1.0         0         0; % Red
1.0       0.6       0; % Orange
0         0.7500    0.7500; % Cyan / Light Blue
0         0.6       0; % Dark Green
%         0.75       0.75       0.2; % Mustard (dark yellow)
%         0          1.0       0; % Bright Green
1.0         0      1.0; % Magenta
%         0.2500    0.2500    0.2500; % Dark Gray
%         0          0       0; % Black
0.6       0.25       0.1]; % Brown

% symlist: Number of entries must equal numel(preheat)
symlist={'o';'x';'s';'*';'^';'d'}; % ;'h';'p'

%% Plot
fig1=figure;
set(fig1, 'Position', [403 49 789 635]);

% % % HUNTS CURVES
% Vector of Solidification Rates
R_val = [0.00045:.0001:0.01-0.0001,0.01:0.1:1-0.1, 1:10:1000]; % cm/s
G_eq=1509.650.*R_val.^(1/2).*(1-2.9348e-4.*R_val.^(-3/2));
G_col=7006.9.*R_val.^(1/2).*(1 - 2.9348e-04.*R_val.^(-3/2));
loglog(R_val,G_col,'--k',R_val,G_eq,'k', 'LineWidth',2);
hold on

% Preheat lines
clear i ct; SymMat=(); ct=1;
pct=length(preheat);
vct=length(Velocity);
for i=1:vct:size(RG,1)  % Plot Preheats
    plot(RG(i:i+vct-1,1),RG(i:i+vct-1,2),'-', ...  
    'Color',[0.50,0.50,0.50],'LineWidth',2)
    SymMat(i:i+vct-1)=symlist(ct); ct=ct+1;
end

% % % Velocity Lines
clear i ct; ColorMat={};
vct=length(Velocity);
for i=vct:-1:1  % Plot Velocity Lines
    plot(RG(i:vct:size(RG,1),1),RG(i:vct:size(RG,1),2),  
    '-','Color',colormat(i,:), 'LineWidth',2)
    ColorMat(i:vct:size(RG,1))={colormat(i,:)};
end

%% Plot points
for m=1:size(RG,1)
    plot(RG(m,1),RG(m,2),char(SymMat(m)),  
    'MarkerEdgeColor',cell2mat(ColorMat(m)),  
    'MarkerFaceColor',cell2mat(ColorMat(m)),  
    'LineWidth',1)
end

%% title(name,'FontSize',16,'FontWeight','bold')
xlabel('Solidification Rate (cm/s)','FontSize',14,'FontWeight','bold')
ylabel('Thermal Gradient (K/cm)','FontSize',14,'FontWeight','bold')

%% If want plot representative point
% hold on
% plot(1.512551597,99133.81753,  
% 'o','MarkerSize',20,'LineWidth',4,'Color',[0.75,0.75,0.2])
% text(1.512551597*2,99133.81753*0.4, 'Representative Point','Color',[0.75,0.75,0.2],'FontSize',13)
% %
xlim([1e-4 1e3]); ylim([1e0 1e6])

set(gca,'linewidth',2,'FontSize',12,'FontWeight','bold');
x_lab=[1e-4,1e-3,1e-2,1e-1,1,le1,le2,le3];
y_lab=[1,le1,le2,le3,le4,le5,le6];
set(gca,'XTick',x_lab,'YTick',y_lab);
axis square
%
% text(2e-4,5e5,'Columnar Grains','FontSize',12,'Color',[0 0 0], ...  
% 'FontAngle','italic','FontWeight','bold')
% text(1e1,7e2,'Equiaxed Grains','FontSize',12,'Color',[0 0 0], ...  
% 'FontAngle','italic','FontWeight','bold')
% text(2e0,5e3,'Mixed Morphology','FontSize',12,'Color',[0 0 0], ...  
% 'FontAngle','italic','Rotation',30,'FontWeight','bold')
% Put Mixed Label at center (le-1,le3); at far right (le1,1.25e4)

%% %**** Legend Box %****
if wantlegend==1;
    r_start=[1.5e-1,1.5]; r_end=[2e2,2e2]; r_size=r_end-r_start;
73
rectangle('Position', [r_start, r_size], 'LineWidth', 2, 'Curvature', 0.2)

% ------------------ COLUMN 1 (POWERS) -------------------------
Col1x = 3e-1; Col12x = 5e-1;
Col1y = [1e2, 5e1, 2.5e1, 1.25e1, 6.5e0, 3.5e0]; % Vertical spacing of Box
for i = 1:pct % for each power
    plot(Col1x(1), Col1y(i), char(symlist(i)), ...
        'MarkerEdgeColor', [0 0 0], 'MarkerFaceColor', [0 0 0], ...
        'LineWidth', 1);
    if length(num2str(preheat(i))) == 4; C2x = Col12x*1.01;
    elseif length(num2str(preheat(i))) == 3; C2x = Col12x*1.35;
    elseif length(num2str(preheat(i))) == 2; C2x = Col12x*1.75;
    end
    text(C2x, Col1y(i), [num2str(preheat(i)), '^oC'], ...
        'FontSize', 12, ...
        'Color', [0 0 0], 'FontWeight', 'bold')
end

% ------------------ COLUMN 2 (VELOCITIES) -----------------------
Col3x = 1.5e1; Col4x = 8e0;
Col3y = [1.2e2, 7e1, 4e1, 2.25e1, 1.25e1, 7.5e0, 4.5e0, 2.5e0];
for i = 1:vct
    if isempty(intersect('.', num2str(Velocity(i)))) ~= 1; % If
        if length(num2str(Velocity(i))) == 4; C2x = Col4x*1.175;
    elseif length(num2str(Velocity(i))) == 3; C2x = Col4x*1.52;
    elseif length(num2str(Velocity(i))) == 2; C2x = Col4x*1.35;
    elseif length(num2str(Velocity(i))) == 1; C2x = Col4x*2.4;
    end
    text(C2x, Col3y(i), [num2str(Velocity(i)), ' mm/s'], ...
        'FontSize', 12, 'Color', colormat(i,:), 'FontWeight', 'bold')
end
else
    fprintf('To generate a legend, change value of variable "wantlegend" to 1\n');
end

C-3.2 Plot Generated by Code

**Figure C-3-1: Solidification Map of Preheat and Velocity Combinations for 500W**
Bibliography


