The Effect of Process Variables on Microstructure in Laser-Deposited Materials

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THE EFFECT OF PROCESS VARIABLES ON MICROSTRUCTURE
IN LASER-DEPOSITED MATERIALS

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy

By

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M.S., Wright State University, 2002

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Abstract

Bontha, Srikanth, Ph.D., Department of Mechanical and Materials Engineering, Wright State University, 2006. The Effect of Process Variables on Microstructure in Laser-Deposited Materials.

Laser deposition of titanium alloys is under consideration for aerospace applications, which require the consistent control of microstructure and resulting mechanical properties. To date, only limited experimental data exists to link deposition process variables (e.g., laser power and velocity) to resulting microstructure (e.g., grain size and morphology) in laser-deposited materials, and suitable microstructures have typically been obtained only by trial and error. In addition, it is unclear whether knowledge based on small-scale laser deposition processes (e.g., LENS™) can be applied to large-scale (higher power) processes currently under development for commercial applications. Therefore, simulation-based methods are needed to predict the effects of process variables and size-scale on microstructure in laser-deposited titanium and other aerospace materials.

The ability to predict and control microstructure in laser deposition processes requires an understanding of the thermal conditions at the onset of solidification. The focus of this work is the development of thermal process maps relating solidification cooling rate and thermal gradient (the key parameters controlling microstructure) to laser deposition process variables (laser power and velocity). The approach employs the well-known Rosenthal solution for a moving point heat source traversing an infinite substrate. Cooling rates and thermal gradients at the onset of solidification are numerically extracted from the Rosenthal solution throughout the depth of the melt pool, and dimensionless process maps are presented for both 2-D thin-wall and bulky 3-D geometries. Results for both small-scale (LENS™) and large-scale (higher power) processes are plotted on solidification maps for predicting trends in grain morphology in laser-deposited Ti-6Al-4V. Although the Rosenthal predictions neglect the nonlinear effects of temperature-dependent properties and latent heat of transformation, a comparison with 2-D and 3-D nonlinear FEM results for both small-scale and large-scale processes suggests that they can provide reasonable estimates of trends in solidification.
microstructure. In particular, both the Rosenthal and FEM results suggest that changes in process variables could potentially result in a grading of the microstructure (both grain size and morphology) throughout the depth of the deposit and that the size-scale of the laser deposition process is important.

In addition, the effects of a uniform distributed heat source on melt pool geometry and microstructure is investigated by superposition of the Rosenthal point source solution. In particular, the effect of beam width on melt pool length, melt pool depth, solidification cooling rates and thermal gradients is investigated. These results are also interpreted in the context of a solidification map to investigate the effect of beam width on trends in grain morphology in laser-deposited Ti-6Al-4V. Finally, transient effects near the free edge are investigated in both 2-D thin-wall and bulky 3-D geometries through thermal finite element analysis. Here the effect of transient melt pool behavior on solidification cooling rates and thermal gradients (and thereby the resulting microstructure) is investigated.
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This dissertation is dedicated to:

Goddess Kanaka Durgamma, my father B. Krishna Mohan Rao and my mother B. Lakshmi
1 Introduction

This dissertation investigates the effects of process variables and size-scale on microstructure in laser-deposited materials, with particular emphasis on laser-based solid freeform fabrication. Solid Freeform Fabrication (SFF) is the name given to a class of manufacturing processes that have evolved from Rapid Prototyping (RP). The naming of the processes as Solid Freeform Fabrication can be explained as follows [1]: The word Solid is used even though the starting state of the material may be a liquid, powder, individual pellets or laminates, since the end output from these processes is a 3D solid object. The word freeform describes the capabilities of these processes to build any complex shapes with few restrictions on their form [1]. As mentioned in [2], these SFF processes have received a lot of attention in the recent past with several books [1,3–14], symposia [15], conferences and numerous conference and journal publications on these processes. These processes have been developed for fabricating complex parts additively in a fast, flexible and automatic manner, without the need for tooling. The SFF processes start with a three-dimensional Computer-Aided Design (CAD) model of an object. This 3-D CAD model is then sliced into 2-D cross-sectional layers by a computer program. The object is then built layer by layer by using any of the available material addition processes (e.g., laser-based deposition processes) [2, 16, 17]. In the early stages of their development, these SFF processes were mainly used for rapid prototyping applications [16, 18]. However, continuous developments in these processes (both process development and the increase in the variety of materials that can be used in these processes) have paved the way for using these processes to fabricate fully dense metal parts for engineering applications [16, 18]. The SFF processes have also found applications in the medical industry [8, 19].

The numerous SFF processes that have been developed are documented in the Solid Freeform Fabrication Symposium Proceedings from 1990 to 2006 [15] and in various books [1, 3–14]. A recent textbook [1] classifies the numerous SFF processes by the starting form of the material. In
this manner they have classified the different processes into (1) liquid-based (2) solid-based and (3) powder-based processes. According to [8] and as mentioned in [2, 17], today there could be at least three or four times that many processes in existence, all at various stages of development. A few of the currently available commercial SFF systems include [1]: 3-D Systems’ Stereolithography Apparatus (SLA), Cubic Technologies’ Laminated Object Manufacturing (LOM), Stratasys’ Fused Deposition Modeling (FDM), 3D System’s Selective Laser Sintering (SLS), Z Corporation’s Three-Dimensional Printing (3DP), Optomec’s Laser Engineered Net Shaping (LENS™), AeroMet Corporation’s Lasform Technology, and Precision Optical Manufacturing’s Direct Metal Deposition (DMD™).

Only the laser-based material deposition processes that are particularly relevant to this dissertation, such as Laser Engineered Net Shaping (LENS™) and Lasform Technology, will be discussed in greater detail.

1.1 Background

This section presents a brief background on the laser-based material deposition processes. Also included in this section is a very brief background on titanium and its alloys, more specifically Ti-6Al-4V.

1.1.1 Laser-Based Material Deposition Processes

The laser-based material deposition processes that are particularly relevant to this dissertation are the Laser Engineered Net Shaping (LENS™) process and AeroMet Corporation’s Lasform Technology.

1.1.1.1 Laser Engineered Net Shaping (LENS™)

The Laser Engineered Net Shaping (LENS™) process was developed at Sandia National Laboratories, and was commercialized by Optomec Design Company in 1997 [1]. The LENS™ process is similar to other SFF processes, in that it is an additive process, where parts are fabricated directly from a 3-D CAD solid model line by line and then layer by layer [20]. The LENS™ system is shown in Figure 1.1 (a). In the LENS™ process, the laser beam creates a molten pool on the
substrate onto which it is focused and powder particles are then injected into the molten pool. A layer is deposited by moving the substrate under the laser beam in the $x$ and $y$ directions. Once the deposition of a layer is completed, the next layer is then deposited by incrementing the powder delivery nozzle and focusing lens assembly in the positive $z$ direction [20, 21]. This layer by layer deposition continues till the part is completed [1]. The fabrication of a thin-wall geometry by the LENS$^\text{TM}$ process is illustrated in Figure. 1.1 (b).

![LENSTM Solid Freeform Fabrication Process](photograph from cover of JOM, Vol.51, No.7, July 1999)

The deposition rates in the LENS process are around 2500 $\text{mm}^3\cdot\text{hr}^{-1}$ [22] or about 0.045 $\text{kg} \cdot \text{hr}^{-1}$ [2, 17]. In this dissertation, the LENS$^\text{TM}$ process is referred to as a small-scale process. This is because the slow deposition rates and relatively low powers ($< 1 \text{ kw}$) in the LENS$^\text{TM}$ process, make it more suitable for the fabrication of small objects. Two of the most commonly fabricated geometries using the LENS process include thin-walled structures and small 3-D deposits.

The LENS$^\text{TM}$ process can be used to fabricate components from a number of metals such as nickel-based super alloys, Titanium alloys particularly Ti-6Al-4V, stainless steels, tool steels and Aluminum alloys [1, 23] Also, the process has been widely used recently to deposit functionally graded materials and composites [24–30].

Lewis and Schlienger [31] compared the tensile properties of laser deposited material with that of conventionally processed material. Their comparison is presented below in table.1.1.
<table>
<thead>
<tr>
<th>Material</th>
<th>0.2 years</th>
<th>UTS</th>
<th>Elong (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MPa (ksi)</td>
<td>MPa (ksi)</td>
<td></td>
</tr>
<tr>
<td><strong>Type 316 stainless steel</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>As deposited</td>
<td>296 (43)</td>
<td>579 (84)</td>
<td>41</td>
</tr>
<tr>
<td>Wrought annealed</td>
<td>262 (38)</td>
<td>572 (83)</td>
<td>63</td>
</tr>
<tr>
<td>Investment cast 316</td>
<td>269 (39)</td>
<td>517 (75)</td>
<td>39</td>
</tr>
<tr>
<td><strong>Inconel 690 (58Ni-29Cr-9Fe)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>As deposited</td>
<td>450 (65.2)</td>
<td>66 (96.6)</td>
<td>48.4</td>
</tr>
<tr>
<td>Hot rolled rod</td>
<td>372 (54)</td>
<td>738 (107)</td>
<td>50</td>
</tr>
<tr>
<td><strong>Ti-6Al-4V</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>As deposited</td>
<td>958 (139)</td>
<td>1027 (149)</td>
<td>6.2</td>
</tr>
<tr>
<td>Wrought bar (annealed)</td>
<td>827-1000 (120-145)</td>
<td>931-1069 (135-155)</td>
<td>15-20</td>
</tr>
<tr>
<td>Cast + anneal</td>
<td>889 (129)</td>
<td>1014 (147)</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 1.1: Tensile Properties of DLF Material Compared to Conventionally Processed Material [31].

1.1.1.2 AeroMet Corporation’s Lasform Technology

AeroMet Corporation’s Laser Forming process [32–40] is similar to LENS™ in operation, in that it is an additive process, where parts are deposited line by line and then layer by layer. However, the deposition rates (4.5 kg/hr−1) [2] and the range of powers (18-30 kW) used in this process are about two orders of magnitude higher than the ones used in the LENS process (0.045 vs. 4.5 kg/hr−1 and 300 vs. 30,000 W). These high deposition rates and laser powers, make the Lasform process more suitable for the fabrication of large bulky deposits. A comparison of select manufacturing factors for the laser forming and conventional manufacturing processes is presented in table.1.2 [37].
AeroMet corporation’s laser forming machine is shown in Figure. 1.2 (a). The machine is a three-axis system [1]. The part is moved by the two-axis table, which provides the motion in the X and Y directions. Movement of the coaxial laser-delivery/powder-nozzle assembly vertically provides the motion in the z direction. The power for the high deposition rates in this laser forming process is provided by the 18 kW CO₂ laser beam [1].

In similarity with the other SFF processes, the AeroMet laser forming process also starts with a 3-D CAD model of the object to be fabricated. As in the LENS™ process, a layer is deposited by moving the substrate below the laser beam in the x and y directions 1.2 (b). The next layer is deposited by moving the laser beam/powder-nozzle assembly upwards in the z direction. This layer by layer deposition is repeated until the object is completely fabricated [1]. The final product
from this process is referred to as a machining preform, which is a near-net-shape part that requires postprocessing (heat treatment, machining and inspection) [1].

![AeroMet Processing Chamber](image1)

![The AeroMet Laser Additive Manufacturing Process](image2)

Figure 1.2: AeroMet’s Laser Additive Manufacturing (a) Chamber (b) Process. [40]

A few examples of the final parts fabricated using this laser forming process are illustrated in Figure. 1.3. AeroMet’s laser forming process has recently been used to deposit Rhenium [41]. Finally, a comparison between AeroMet’s laser forming process and LENS™ process is presented in Figure. 1.4 [2].

![Machined LAM Ti-6Al-4V Parts](image3)

Figure 1.3: Machined LAM Ti-6Al-4V Parts. From Bottom Left Counter Clockwise: Cylindrical Geometries, Aircraft Fitting and Angled walls [40]
<table>
<thead>
<tr>
<th>Parameter</th>
<th>LasForm</th>
<th>LENS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laser</td>
<td>18 kW Continuous CO₂</td>
<td>1-2 kW Nd:YAG</td>
</tr>
<tr>
<td>Powder Delivery</td>
<td>High-Mass Rate Powder Feed, single axis</td>
<td>Powder Feed, multi-axis</td>
</tr>
<tr>
<td>Chamber Size</td>
<td>12(\times) 4(\times) 4(\text{ft} \times 1.2(\text{m}) \times 1.2(\text{m}))</td>
<td>1.5(\times) 1.5(\times) 3.5(\text{ft} \times 0.46(\text{m}) \times 1.07(\text{m}))</td>
</tr>
<tr>
<td>Work Table Capacity</td>
<td>20,000 pounds [9 tons]</td>
<td>20,000 pounds [9 tons]</td>
</tr>
<tr>
<td>Atmosphere</td>
<td>Dynamically Purged with high purity Argon, (&lt; 150 ppm O₂)</td>
<td>Argon</td>
</tr>
<tr>
<td>Deposition Rate</td>
<td>2.0 - 9.9 lb(\text{hr}^{-1}) ([0.90 - 4.5 \text{kg hr}^{-1}])</td>
<td>0.1 lb(\text{hr}^{-1}) ([0.045 \text{kg hr}^{-1}])</td>
</tr>
<tr>
<td>Powder</td>
<td>Pre-Alloyed, Blended Elemental +325 mesh, Graded Capability</td>
<td>Pre-Alloyed, Blended Elemental, Graded Capability</td>
</tr>
<tr>
<td>Near, Net Shape (Oversize)</td>
<td>Near-Net ((0.03 - 0.2 \text{ in} \times 0.762 - 5.08 \text{mm}))</td>
<td>Net</td>
</tr>
<tr>
<td>Reproducibility</td>
<td>±0.03 in ([±0.76 \text{ mm}])</td>
<td>±0.005 in ([±0.127 \text{ mm}])</td>
</tr>
<tr>
<td>Layer Dimensions</td>
<td>([≥15\times 8 \text{ mm}])</td>
<td>([≥1\times 2 \text{ mm}])</td>
</tr>
<tr>
<td>Typical Products</td>
<td>Small to Large Structural Parts</td>
<td>Small Structural Parts, Tooling</td>
</tr>
</tbody>
</table>

Figure 1.4: Comparison Between AeroMet’s Lasform Technology and LENS™ processes [2]

In this dissertation, the AeroMet’s Lasform Technology is referred to as large-scale or higher power process. This is because as discussed previously, the high deposition rates and laser powers, make it more suitable for the fabrication of large bulky deposits. The range of laser velocities used in AeroMet’s laser forming process is comparable to that used in small-scale (LENS) process i.e., on the order of 5-25 inches/minute. However, the range of laser powers used in AeroMet’s laser forming process (upto 30,000 W ) can be higher by as much as two orders of magnitude when compared to the range used in the small-scale (LENS) process. Therefore, most of the discussion in this dissertation on the effects of size-scale will focus primarily on laser power. It should finally be noted that there are other "mid-scale" processes under development, including the one at the Advanced Materials Processing (AMP) Center of South Dakota School of Mines and Technology with laser powers of about 3 kW.

1.1.2 Titanium Alloys

Titanium was first discovered in 1790 by W. Gregor (England) and M.H. Klaproth (Germany) [42]. Titanium is the ninth most abundant element of the earth’s crust and fourth most abundant of the structural metals [42, 43]. The properties of titanium that make it attractive for many industries (especially the aerospace industry) are high strength, low density, good high temperature properties
and excellent corrosion resistance. The introduction of titanium to the aerospace industry took place in the 1950’s. A few of the non-aerospace applications of titanium include steam-turbine blades, hydrogen-storage media and high-current/high-field superconductors [42].

The most common and widely used titanium alloy is Ti-6Al-4V. The uniqueness of Ti-6Al-4V is that it combines attractive properties with inherent workability and good shop fabricability [44]. Ti-6Al-4V is most widely used in the aerospace industry. The titanium alloy that is most relevant to this dissertation is Ti-6Al-4V.

1.1.2.1 Composition of Ti-6Al-4V

The product forms in which Ti-6Al-4V is available are wrought, cast and powder metallurgy (P/M) forms [44]. The primary alloying elements in Ti-6Al-4V are Aluminum (Al) and Vanadium (V), with small amounts of Oxygen (O) and Nitrogen (N) [44].

1.1.2.2 Titanium Microstructure

The primary motivation of this research is to investigate the effects of key laser deposition process variables (e.g., laser power and velocity) and size-scale on solidification microstructure (grain size and morphology). In this dissertation, the term "microstructure" actually refers to the macrostructure (grain size and morphology) of the material. Trends in grain size and morphology are investigated for different processing conditions (changes in laser power or velocity) specifically for the Ti-6Al-4V material system. The effect of microstructural features on mechanical properties in titanium alloys is summarized in table 1.3. More information on structure-property relationships that exist in titanium alloys can be found in the work of Flower [45] and Lutjering [46].
<table>
<thead>
<tr>
<th>Feature</th>
<th>Enhances</th>
<th>Degrades</th>
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<tbody>
<tr>
<td>Elongated $\alpha$</td>
<td>Fracture Toughness</td>
<td>Ductility</td>
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<td></td>
<td>Notched Fatigue Resistance</td>
<td>Fatigue Initiation Resistance</td>
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<td></td>
<td>Fatigue Crack Growth Resistance</td>
<td>Low Cycle Fatigue Resistance</td>
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<tr>
<td>Widmanstatten $\alpha$</td>
<td>Fracture Toughness, Creep</td>
<td>Ductility, Strength</td>
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<td></td>
<td>Notched Fatigue Resistance</td>
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<td>Fatigue Crack Growth Resistance</td>
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<td>Bi-Modal $\alpha$</td>
<td>Strength, Ductility</td>
<td>Fatigue Crack Growth Resistance</td>
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<td>Fatigue Initiation Resistance</td>
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<td>Low Cycle Fatigue Resistance</td>
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<td>Colony $\alpha$</td>
<td>Fatigue Crack Growth</td>
<td>Strength, Ductility</td>
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<td>Fracture Toughness</td>
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<td></td>
<td>Notched Fatigue Resistance</td>
<td>Low Cycle Fatigue Resistance</td>
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<tr>
<td>Secondary $\alpha$</td>
<td>Strength, Ductility</td>
<td>Fatigue Initiation Resistance</td>
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<tr>
<td>Grain Shape (elongated)</td>
<td>Fracture Properties</td>
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<td>Fatigue Crack Growth Resistance</td>
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<td>Notched Fatigue Resistance</td>
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<td>Coarse Prior $\beta$ Grains</td>
<td>Fracture Toughness</td>
<td>Strength, Ductility</td>
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<td>Creep</td>
<td>Fatigue Initiation Resistance</td>
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<td>Fine Prior $\beta$ Grains</td>
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<td>Strength, Ductility</td>
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<tr>
<td>Grain Boundary $\alpha$</td>
<td>Fracture Toughness</td>
<td>Ductility, Fatigue Initiation Resistance</td>
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<td>Fatigue Crack Growth</td>
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<td></td>
<td>Notched Fatigue Resistance</td>
<td>Low Cycle Fatigue Resistance</td>
</tr>
</tbody>
</table>

Table 1.3: Morphology-Property Relationship in Titanium Alloys [47].

The current dissertation focuses on the solidification microstructure, including the size and morphology of the prior $\beta$ grains (equiaxed or columnar). Solid state phase transformations have not been investigated, and are left for subsequent researchers.

### 1.2 Motivation, Objectives and Approach

As discussed previously, laser-based solid freeform fabrication is a novel manufacturing process in which a solid metallic object can be fabricated directly from a three-dimensional CAD representation of the object. Right from the time of their initial development, the laser-based SFF processes such as LENS™ and Lasform Technology have proved beyond doubt that they can be useful manu-
facturing techniques. However, the primary obstacles to the widespread commercialization of these processes as viable manufacturing alternatives for metallic components include the control of melt pool size, residual stress and microstructure [16]. The control of melt pool size and residual stress in these processes have recently been addressed in the literature [18, 48–51], while the control of microstructure has not yet been addressed.

Laser deposition of titanium alloys is under consideration for aerospace applications. As stated in [52–55], application of laser deposition processes for the fabrication of titanium aerospace components substantially reduces both the buy-to-fly ratio and the lead time for production, two factors which effect cost. At the same time, the properties of the components fabricated by these laser-based processes are similar to those fabricated using conventional manufacturing processes. All these factors are responsible for propelling these laser deposition processes as an attractive choice for the fabrication of titanium aerospace components.

That said, the widespread use of this promising technology will ultimately depend on the ability to predict and control the microstructure and the resulting mechanical properties of the deposit [56]. The control of microstructure and the resulting mechanical properties assumes critical importance when these laser deposition processes are used for the fabrication of aerospace components, because of the strict guidelines aerospace applications have on microstructure and mechanical properties. To date, most of the progress in relating laser deposition process variables (e.g., laser power and velocity) to the resulting microstructure (e.g., grain size and morphology) has been limited experimentation coupled with intuition [52,54,57–59], and suitable microstructures have typically been obtained only by trial and error. Therefore, simulation based methods are needed for understanding the effects of the key laser deposition process variables on the resulting microstructure in laser deposited materials. In addition, it is also unclear as to whether the gained microstructural knowledge based on small-scale laser deposition processes (e.g., LENS™) can be applied to large-scale (higher power) processes (e.g., AeroMet’s process). The current research tries to address both the effects of process variables (laser power and velocity) and size-scale on solidification microstructure in laser deposited materials through a combination of analytical and numerical modeling approaches. The material system selected in this dissertation for the above investigations is Ti-6Al-4V, as it is widely used in aerospace applications.

In this dissertation, the analytical approach is based on the well known Rosenthal solution for
a moving point heat source traversing an infinite substrate [60], which has been used recently in the literature to guide the development of process maps relating laser deposition process variables to melt pool size and residual stress [18, 48–51]. In this research the Rosenthal solution is used to develop previously unreported thermal process maps for solidification cooling rates and thermal gradients (the key parameters controlling microstructure). Cooling rates and thermal gradients at the onset of solidification are numerically extracted from the Rosenthal solution throughout the depth of the melt pool, and dimensionless process maps are developed for both, 2-D thin-walled structures and bulky 3-D deposits. The developed thermal process maps relate the key laser deposition process variables (laser power and velocity) to solidification cooling rates and thermal gradients (the key parameters controlling microstructure). The results from the developed process maps are then used to provide general insights into the roles of process variables and size-scale on solidification microstructure, in particular for the Ti-6Al-4V material system. Since the Rosenthal solution assumes temperature-independent properties, the thermal process maps that have been developed using the Rosenthal solution can therefore be applied to any material system.

The nonlinear effects of temperature-dependent properties and latent heat that are neglected by the Rosenthal solution are then investigated through thermal finite element modeling. In this research, the primary purpose of the finite element modeling is to assess the validity of the Rosenthal results for predicting trends in solidification microstructure. This has been investigated for small-scale (LENS™) deposition of thin-walled structures and both small-scale (LENS™) and large-scale (higher power) deposition of bulky 3-D deposits. Numerical results obtained from both Rosenthal and FEM solutions are plotted on solidification maps [53, 55, 56, 58, 61, 62] for predicting grain morphology in Ti-6Al-4V, and the utility of the Rosenthal solution is discussed.

In both the Rosenthal and FEM modeling, laser deposition processes are considered on two different scales: small-scale and large-scale. Small-scale processes are typically referred to as LENS™ and will be investigated for both the deposition of thin-walled and bulky deposits over the LENS™ range of laser powers and velocities. Large-scale or higher power processes will be investigated for the deposition of only bulky structures. In the large-scale processes, the range of laser velocities considered is exactly the same as the range considered for small-scale (LENS™) processes. This is because the range of laser velocities considered in both small-scale and large-scale processes are comparable (5-25 inches/minute). However the range of laser powers considered in the large-scale
processes spans 5-30 kW, which is up to two orders of magnitude larger than typical LENS\textsuperscript{TM} powers.

One of the limitations of both the analytical and numerical modeling approaches used in this dissertation is that they do not account for powder deposition. This dissertation takes the first basic step of investigating the previously unreported results on the effects of process variables and size-scale on solidification microstructure in laser deposited materials. However, the trends in solidification microstructure for Ti-6Al-4V predicted by the analytical and numerical modeling approaches herein, are in agreement with the experimental results reported for actual laser deposition of Ti-6Al-4V.

1.3 Literature Review

1.3.1 Laser Deposition of Titanium

Research on laser deposition of titanium alloys, has received a lot of attention in the last decade, and several papers have been published which discuss the microstructure and mechanical properties of laser-deposited titanium alloys [17, 32–34, 36–39, 52–55, 58, 59, 63–67]. The initial research in this area was aimed at developing a laser based rapid manufacturing process for titanium and titanium alloys [32]. The developed process was initially referred to as LaserCas\textsuperscript{TM} and later became AeroMet’s Lasform\textsuperscript{SM} process. Most of the papers emanating from this research [32–35,37–39] discussed about the advantages of the Lasform\textsuperscript{SM} process over the conventional manufacturing methods. An initial study on the production economics [32, 33] of two different titanium parts produced by the Lasform\textsuperscript{SM} process indicated that titanium parts can be delivered at 50 % or less cost compared to similar parts produced by conventional manufacturing processes. The study also indicated a 50 % or more reduction in the delivery times with the Lasform\textsuperscript{SM} process. Again most of the papers, also provide information on the development of equipment and process parameters, along with the test results of dimensional stability, ultrasonic inspection, chemical analysis, metallographic inspection and mechanical testing conducted on parts produced by the Lasform\textsuperscript{SM} process. Further most of these papers, also reported mechanical properties equivalent to or in few cases exceeding those obtained from conventional manufacturing processes. Another study, that investigated the mechanical properties of laser-deposited titanium parts was carried out by Kobryn and Semiatin [52]. Here, the mechanical properties of Ti-6Al-4V parts deposited using the Laser Engineered Net Shaping
process were investigated. This research focused on the effect of porosity and texture on the mechanical properties (tensile properties, fatigue strength and fracture toughness) of bulky Ti-6Al-4V deposits fabricated using the LENSTM process. The work clearly illustrated the negative effect of porosity on the mechanical properties and the need to eliminate porosity in order to improve the mechanical properties of laser fabricated Ti-6Al-4V. Despite, all this extensive research on equipment development and mechanical property investigation, very limited work was reported on the relationship between the deposition process variables and the deposit structure.

Brice et al., [57] conducted an initial study to investigate the effect of process parameters on the quality of the Ti-6Al-4V parts deposited using the LENS system. In this work, the effect of traverse speed, laser power, powder flow rate, layer thickness, hatch width and stand-off distance on the deposited samples (build height and porosity) was investigated using a screening design of experiments method. This work reported that powder flow rate needs to be monitored carefully to obtain an acceptable deposit and that stand-off distance need not be considered as a process variable.

Another work that investigated the effect of process parameters (laser power and traverse speed) on microstructure, porosity and build height was carried out by Kobryn et al., [54]. Here too, the LENS system was used to fabricate Ti-6Al-4V deposits for the investigation. This work reported a columnar macrostructure and a fine Widmanstätten microstructure in all the deposits. A macroscopic banding was also reported in all the specimens, which was reasoned by the authors as due to the reheating of the already deposited layer when depositing subsequent new layers. The work also reported a decrease in the two types of porosity observed in the deposits (lack-of-fusion porosity and gas porosity) with increasing laser power and velocity. The conclusions on the effect of process parameters on build height was that increasing speed decreases build height, while the effect of power on build height is not very clear.

Kobryn et al., [53, 55, 58] also carried out a study to investigate the range of microstructures obtained in laser-deposited Ti-6Al-4V. In this study, in addition to laser power and velocity, they also considered laser spot size/shape as another variable. For this study, Ti-6Al-4V deposits were made using two different laser systems. The first one was a low power Nd-YAG laser system (LENS) with a ~1 mm diameter circular beam and a Gaussian intensity distribution, while the second one was a high power CO2 laser system with a ~13 mm square beam and a uniform intensity distribution. The Ti-6Al-4V deposits from the two different laser systems were then examined for

13
size and morphology of prior $\beta$ grains and also the transformed microstructure. The macro and microstructures of the deposits from the Nd-YAG system were similar to that reported in [54]. The macrostructure of the CO$_2$ deposit was also columnar, while the microstructure of the CO$_2$ deposit had a coarser widmanstätten morphology. A macroscopic bonding as reported in the authors other work [54], was also observed here in the CO$_2$ deposits. This study also reported that the grain size decreased with increasing traverse speed, while laser power did not significantly affect grain size.

In a very recent study, Wu et. al., [59], experimentally investigated the effect of deposition process variables: laser power, velocity and powder feed rate on the resulting microstructure in thin-wall Ti-6Al-4V deposits. For this study, the thin-wall samples were deposited using a 1750 W CO$_2$ laser system. This work reported that increasing laser power results in a transition from columnar to mixed/equiaxed morphology, and increasing velocity results in a decrease in grain size. The work also reported the presence of layer bands and concludes that the grain morphology in laser-deposited thin-wall Ti-6Al-4V deposits is strongly influenced by directional solidification.

Kelly and Kampe [66, 67] carried out a study to understand the evolution of microstructure in laser-deposited Ti-6Al-4V builds using both experimental [66] and modeling approaches [67]. In the experimental study [66], they examined an eighteen layer Ti-6Al-4V deposit fabricated using AeroMet’s laser forming process. This work also reported a macrostructure with columnar prior $\beta$ grain morphology. Macroscopic bands were also reported for all layers except the last three. The authors reasoned that the macroscopic bands were owing to the complex thermal history experienced by the deposit.

1.3.2 Thermal Conditions in the Laser Deposition Process

Right from the time of its initial development at Sandia National Laboratories, continuous research on the LENS™ process [20–24, 63, 68–93] has not only helped the process to be seen as a very promising manufacturing technique, but has also greatly contributed towards understanding the thermal conditions [72, 80, 81, 83, 84, 86, 89] in the laser-based material deposition processes. A thorough understanding of the thermal conditions (cooling rates and thermal gradients) at the onset of solidification is also needed to predict and control microstructure in laser deposition processes.

Griffith et al., [81] carried out a study to understand the thermal behavior in the LENS™ process. In this study they measured the temperatures using thermocouple measurements, infrared imaging
and high speed visible imaging. The goal of this study was to use the measured thermal signatures for developing a real time feedback control system for the LENS™ process. Hofmeister et. al., [80, 84, 86] have in a study tried to understand the thermal behavior in the LENS™ process by coupling thermal measurements with finite element modeling and microstructural analysis. In this study, the cooling rates and thermal gradients were obtained from the thermal images of the melt pool.

A study that investigated the thermal behavior in the LENS™ process using both experimental and finite element modeling approaches was carried out by Wei et. al., [89, 94]. In this study, a two-wavelength imaging pyrometer system was used for recording the thermal images. The thermal behavior was investigated for different values of laser power and velocity. Both stationary melt pools (size and shape) and moving melt pools (thermal history) were characterized in this work. Finite element modeling [89] was used for analyzing the complete thermal behavior (temperature distribution and thermal gradients) during the part fabrication.

In a very recent study, Unocic and DuPONT [92] investigated the effects of laser power, velocity and powder flow rate on the laser beam energy absorbed by the substrate. For the purposes of this study, single pass deposits of H-13 steel and copper were made on H-13 steel substrates. For investigating the effects of process variables on the process efficiencies, three dimensionless process efficiencies: laser energy transfer efficiency, melting efficiency and deposition efficiency were measured. The study reported that the range of laser energy transfer efficiency was between 30 to 50 pct while the maximum value of deposition efficiency was ~ 14 pct. The work also reported an increase in the melting efficiency with increasing the three process variables considered in the study.

1.3.3 Thermal Modeling of the Laser Deposition Process

A considerable amount of work has been reported in the literature [16–18, 48–51, 56, 61, 62, 67, 73, 75, 76, 80, 89, 94–107] on developing both analytical and numerical models for understanding various process related issues in laser-based material deposition processes. However, only a few researchers and that too very recently [17, 53, 56, 58, 62, 67, 80, 103, 107] have used simulation-based methods for understanding microstructure related issues in laser-based material deposition processes.

Vasinonta et. al., [18, 48–51] have developed process maps that relate deposition process variables to melt pool size and residual stress. These process maps have been developed employing
the analytical Rosenthal solution in conjunction with thermomechanical finite element modeling
and have been developed for both 2-D thin-walled and bulky 3-D geometries. The developed pro-
cess maps contain results from simulations with both temperature-independent and temperature-
dependent properties. This research reported a reduction in residual stresses by preheating the base
plate and that the small increases if any in the size of the melt pool due to the preheating of the base
plate can be controlled by minor changes in laser power or velocity.

Kobryn et.al., [53, 55, 58], in addition to their work on the effect of process variables on mi-
crostructure and build characteristics, also conducted finite element simulations of single pass laser
glazes using the ProCAST\textsuperscript{TM} software for two different laser systems (low-power Nd-YAG and
high power CO\textsubscript{2} systems). In order to validate the numerical simulation results they made single
pass experimental laser glazes using both the Nd-YAG and CO\textsubscript{2} laser systems. The FEM pre-
dicted size and shapes of the fusion and heat affected zones were compared with the measured ones.
Also, the numerical data of thermal gradients ($G$) and solidification velocity ($R$) from the FEM
simulations was plotted on the solidification map of Ti-6Al-4V to predict the grain morphology in
laser-deposited Ti-6Al-4V. The Solidification map predicted grain morphology was also compared
with the experimental glaze morphology. Both the FEM and experimental results revealed that the
grain morphology from the Nd-YAG laser glazes was columnar while the morphology from the CO\textsubscript{2}
laser glazes was mixed.

More recently, Brown [17], proposed an approach for modeling solidification microstructure in
laser deposition of thin-wall Ti-6Al-4V structures. Brown in his work proposed coupling thermal
finite element modeling with Cellular Automaton (CA) modeling of solidification microstructure.
The 3-D thermal finite element modeling was carried out using the software package ProCas\textsuperscript{TM},
while the 3-D Cellular Automaton modeling was carried out using the software package CAFE3D\textsuperscript{TM}.
This work also investigated the Ti-6Al-4V solidification parameters that are needed for CA mod-
eling of solidification microstructure. The work also calibrated the fraction of the absorbed laser
power to be $\alpha = 0.35$, for LENS\textsuperscript{TM} deposition of thin-wall Ti-6Al-4V deposits. The simulated mi-
crostructures from the proposed modeling approach were compared with experimental microstruc-
tures and the results were [17] found to be in good agreement.

Hofmeister \textit{et. al.}, [80] created preliminary finite element models using the element birthing
technique to simulate the thermal behavior during the fabrication of thin-wall stainless steel parts
using the LENS™ process. Labudovic et. al., [98] developed a three-dimensional finite element model with the element birthing technique using ANSYS to understand the temperature and residual stress distribution in thin-wall parts fabricated using the laser deposition process. The FEM calculated residual stresses were compared with that calculated using x-ray diffraction technique and were found to be in good agreement. Kelly and Kampe [67] in conjunction with their experimental work on understanding the evolution of microstructure in laser-deposited Ti-6Al-4V multilayer builds [66] also developed a thermal model to understand the complex thermal history experienced by the build during the deposition process. Another model to predict microstructural evolution in laser-deposited multilayer tool steel builds was presented by Costa et. al., [103]. This model coupled thermal FEM and transformation kinetics to simulate the evolution of microstructure.

In a very recent work, Gaddam [107] extended the modeling approach proposed by Brown [17] to both small-scale and large-scale deposition of bulky Ti-6Al-4V deposits. This work also addressed some of the limitations of Brown’s work i.e., considering a curvilinear shape for the melt pool instead of the rectangular shape as considered by Brown and also applying melt pool boundary conditions that simulate a three dimensional heat transfer instead of the conditions that simulated a one dimensional heat transfer in the work by Brown. In this work, an alternative approach to modeling solidification microstructure was also proposed. Here, the thermal history that was needed for microstructure modeling was obtained from the analytical 3-D Rosenthal solution instead of from the ProCAST™ thermal finite element model. This new approach was then used to investigate the effects of process variables (laser power and velocity) and size-scale (low power vs. higher power processes) on solidification microstructure in laser fabricated bulky 3-D Ti-6Al-4V deposits. This work also validated the solidification map predictions for both small-scale and large-scale deposition of bulky 3-D geometries presented in this dissertation.

1.4 Contributions of this Research

Despite the continuous research and development of the laser-based material deposition processes both experimentally and numerically, there are still issues that need to be addressed. Some of the issues regarding these processes that are not well known are:

- The effects of key deposition process variables on microstructure in laser-deposited materials.
To date, suitable microstructures for particular build geometries have typically been obtained through trial and error, and only limited experimental data exists to relate the obtained microstructure with the deposition process variables.

- The role of size-scale. This is because laser-based material deposition processes encompass a wide range of size scales (from a 300-800 W laser system used in the LENS process, to a 3 kW laser system currently under development at South Dakota School of Mines and Technology, and finally to a, 18 kW laser system being used in AeroMet’s laser forming process). The size-scale of the process has a direct effect on the cooling rates and thermal gradients and potentially the resulting microstructure. The point that is unclear here is whether or not the knowledge on microstructure gained from working with small-scale processes (e.g., LENS™) can be applied to the large-scale processes currently under development for commercial application.

- The effect of melt pool behavior near a free edge on solidification cooling rates and thermal gradients (and thereby on the resulting microstructure).

- The effect of laser beam width and shape on melt pool length, melt pool depth and microstructure in laser-fabricated structures.

Addressing the current lack of understanding on the above issues forms the basis of this research. The thermal process maps for solidification cooling rates and thermal gradients developed in this research provide a crucial link between the deposition process variables and the resulting microstructure. In this dissertation, the two basic geometries that have been considered are the 2-D thin-walled structures and bulky 3-D deposits. Moreover, as the process maps are developed assuming temperature-independent material properties, they can be applied to any material system.

In brief, the contributions of this research are:

- Development of previously unreported thermal process maps for dimensionless solidification cooling rates and thermal gradients for both 2-D thin-walled and bulky 3-D structures. Based on the Rosenthal point source solution, these process maps fully map out the effects of the key laser deposition process variables (laser power and velocity) and size-scale on solidification microstructure in laser-deposited materials.
• Demonstration of the utility of the Rosenthal solution for predicting trends in solidification microstructure for both small-scale and large-scale processes.

• Further underscoring the utility of the solidification map approach for predicting trends in grain morphology in laser-processed materials, particularly Ti-6Al-4V.

• Presentation of previously unreported results for the effect of melt pool behavior on solidification cooling rates and thermal gradients (and thereby on the resulting microstructure) in the vicinity of the free edge.

• Presentation of previously unreported formulations for a uniform distributed heat source in both 2-D and 3-D based on the superposition of the 2-D and 3-D Rosenthal solution point source solution.

• Presentation of previously unreported results for the effect of laser beam width and shape on melt pool length, melt pool depth, solidification cooling rates, thermal gradients and finally on the resulting microstructure in the Ti-6Al-4V material system.

1.5 Organization of the dissertation

The development of thermal process maps for solidification cooling rates and thermal gradients using the analytical Rosenthal solution for a moving point heat source is discussed in chapter 2. The process map development is presented for 2-D thin-walled geometries and bulky 3-D deposits. These two represent the geometries that are most commonly fabricated using the laser-based SFF processes. Chapter 2 begins with details of the Rosenthal 2-D and 3-D solutions, and their dimensionless forms in terms of the process variables of interest. The procedures by which the process maps for solidification cooling rates and thermal gradients are developed are then described in detail. Finally, these process map results are interpreted in the context of a solidification map for predicting trends in solidification microstructure in Ti-6Al-4V, for both small-scale (LENS™) and large-scale (higher power) processes.

Chapter 3 includes the nonlinear effects of temperature-dependent properties and latent heat through thermal finite element analysis. First, the details of the 2-D finite element modeling are
provided. These details include the element type, boundary conditions and information on approximating the laser deposition process as a moving point heat source. Then the procedures for extracting the cooling rates and thermal gradients at the onset of solidification throughout the depth of the melt pool are presented. Next, the details of 3-D finite element modeling are presented. These details include the element type, boundary conditions, and a rigorous convergence study. Next, a comparison between the FEM and Rosenthal results is interpreted in the context of the solidification map, for Ti-6Al-4V, for both small-scale and large-scale processes. Finally, the utility of the Rosenthal solution for predicting trends in solidification microstructure is discussed.

Chapter 4 presents the effects of melt pool behavior in the vicinity of a free edge on solidification cooling rates and thermal gradients and thereby on the resulting microstructure in the Ti-6Al-4V material system through thermal finite element analysis of both 2-D thin-wall and bulky 3-D geometries. First the 2-D modeling approach is briefly outlined. Next, the nondimensionalization scheme used for presenting results from simulations run with temperature-independent properties is discussed. Results illustrating the effect of melt pool behavior on solidification cooling rates and thermal gradients in 2-D thin-wall geometries are presented next for two different cases. In the following section, results from simulations with temperature-dependent material properties for Ti-6Al-4V are interpreted in the context of a solidification map to understand the effect of melt pool behavior on trends in grain morphology in laser-deposited Ti-6Al-4V. Finally, the effects near the free edge in bulky 3-D geometries is presented. Here again, the modeling approach, nondimensionalization scheme used for presentation of temperature-independent simulation results, and the results from simulations run with temperature-independent and temperature-dependent material properties for Ti-6Al-4V are presented.

Chapter 5 presents the effects of beam width and shape on melt pool length, melt pool depth, solidification cooling rates, thermal gradients and microstructure in both 2-D thin-wall and bulky 3-D geometries through superposition of the 2-D and 3-D Rosenthal point source solution respectively. First, the formulation for a uniform distributed heat source in 2-D that is obtained by the superposition of the 2-D Rosenthal point source solution is presented. The next section presents results that illustrate the effect of beam width on melt pool length, depth, solidification cooling rates and thermal gradients. The effect of beam width on trends in grain morphology in laser-deposited Ti-6Al-4V is illustrated next through a solidification map. The following sections present the for-
ulations for a uniform distributed heat source with both circular and square beam profiles through superposition of the 3-D Rosenthal point source solution. Finally, the effect of beam width and shape on melt pool length, depth, solidification cooling rates, thermal gradients and microstructure in laser fabricated bulky 3-D structures is presented for both small-scale (LENS™) and large-scale (higher power) processes.

Chapter 6 presents the summary and once again reiterates the major contributions of this dissertation.

Chapter 7 lists the tasks that have been identified as future research directions.
2 Thermal Process Maps Based on Rosenthal Solution for a Moving Point Heat Source

2.1 Introduction

In 1946, Rosenthal proposed the theory of heat flow due to a moving source [60]. He derived solutions for linear, two and three-dimensional flow of heat in both infinite and semi-infinite solids. The Rosenthal solution assumes temperature-independent thermophysical properties.

The Rosenthal point source solution was initially applied to welding [108–112]. Application of the Rosenthal point source solution to the laser deposition process was first carried out by Dykhuizen and Dobranich [73,75,76]. They used the Rosenthal 2-D and 3-D point-source conduction solutions for coming up with analytical models for the LENS™ process [76]. In this work, the Rosenthal solution was also used for coming up with analytical expressions that would help in understanding the sensitivity of the cooling rates to changes in laser power and velocity [75]. Vasinonta and Beuth [18, 48–51] have employed the Rosenthal point source solution to identify the dimensionless process variables governing thermal conditions in laser deposition processes. By using the Rosenthal solution in conjunction with thermal finite element modeling they have developed non-dimensionalized plots termed as “process maps” which relate deposition process variables to melt pool size and residual stress in both thin-wall (2-D) and bulky (3-D) geometries.

In this dissertation, a similar approach as employed by Vasinonta and Beuth is used to investigate solidification cooling rates and thermal gradients (the key parameters controlling microstructure) in laser deposition processes. Cooling rates and thermal gradients at the onset of solidification are
numerically extracted from the Rosenthal solution throughout the depth of the melt pool, and dimensionless process maps are developed for both 2-D and 3-D geometries. In addition, superposition of the Rosenthal point source solution is also carried out to investigate the effects of beam width and shape (circular vs. square laser beam with a uniform intensity distribution).

This chapter presents the process map development using the analytical Rosenthal solution. Process map development will be presented for two basic geometries as shown in figures 2.1 and 2.2. Thin-walled geometries (Figure 2.1) and bulky geometries (Figure 2.2) of this type are commonly fabricated using the LENS™ and other laser-based solid freeform fabrication processes. For both the geometries, it is assumed that the length \( L \) and height \( h \) are sufficiently large such that the steady-state Rosenthal solution for a moving point source on an infinite half space applies. In Figs. 2.1 and 2.2, the variables \( \alpha Q \) and \( V \) represent the fraction of the absorbed laser power and the laser velocity respectively. These two are the key process variables, whose effects on microstructure will be investigated as part of this research. Finally, the relative coordinates \( (x_0, y_0, z_0) \) in Figs. 2.1 and 2.2 are related to the fixed spatial coordinate \( (x, y, z) \) at any time \( t \) as \( (x_0, y_0, z_0) = (x - Vt, y, z) \), where \( V \) is the velocity.

![Figure 2.1: Thin-Wall Geometry](image-url)
2.2 Process Map Development for 2-D Thin-Walled Geometries

The Rosenthal point source solution for two-dimensional flow of heat in a semi-infinite thin plate (Figure 2.1) is given as [60]

\[ T - T_0 = \frac{\alpha Q}{\pi k b} e^{-\lambda V x_0} K_0(\lambda V r). \] (2.1)

In equation (2.1) \( \alpha Q \) is the absorbed laser power, \( V \) is the speed of the source, \( T \) is the temperature at a location relative to the moving point source, \( T_0 \) is the initial temperature of the solid, \( b \) is the thickness of the plate, \( K_0 \) is the modified Bessel function of the second kind and order zero, \( k \) is the thermal conductivity, \( r = \sqrt{x_0^2 + z_0^2} \) is the radial distance from the heat source and \( 1/2\lambda \) is the thermal diffusivity of the metal. If \( \rho \) is the mass density and \( c \) is the specific heat of the metal then \( \lambda = \frac{\rho c}{2k} \).

Vasinonta and Beuth presented the Rosenthal 2-D solution in dimensionless form [18, 48–51] as

\[ \mathcal{T} = e^{-\gamma x_0} K_0(\sqrt{x_0^2 + z_0^2}). \] (2.2)

The dimensionless variables in equation (2.2) are defined in terms of the process variables of interest, i.e., absorbed laser power \( \alpha Q \) and velocity \( V \)

\[ \mathcal{T} = \frac{T - T_0}{\alpha Q/\pi k b}, \quad x_0 = \frac{x_0}{\frac{2k}{\rho c V}}, \quad z_0 = \frac{z_0}{\frac{2k}{\rho c V}}. \] (2.3)

In equation (2.3) \( T \) is the temperature at a location \((x_0,z_0)\) relative to the moving point source (Fig. 2.1), \( T_0 \) is the initial temperature of the wall, \( \rho \), \( c \) and \( k \) are the density, specific heat and
thermal conductivity of the material respectively. The relative coordinates \((x_0, z_0)\) at any time \(t\) are related to the fixed spatial coordinate \((x,z)\) as \((x_0,z_0) = (x - Vt, z)\).

As previously discussed, the parameters of interest in controlling microstructure are solidification cooling rate and thermal gradient. The expressions for the dimensionless cooling rate and thermal gradient and can be obtained through differentiation of equation (2.2). The expression for dimensionless cooling rate is given by equation (2.4) and the expression for dimensionless thermal gradient is given by equation (2.7).

\[
\frac{\partial T}{\partial \tau} = e^{-\tau} \left\{ \frac{(\tau - 1)}{\sqrt{(\tau - 1)^2 + \xi_0^2}} \right\} K_1 \left( \sqrt{(\tau - 1)^2 + \xi_0^2} \right) + K_0 \left( \sqrt{(\tau - 1)^2 + \xi_0^2} \right),
\]

(2.4)

\[
\frac{\partial T}{\partial \xi_0} = -e^{-\xi_0} \left\{ \frac{\xi_0}{\sqrt{\xi_0^2 + \xi_0^2}} \right\} K_1 \left( \sqrt{\xi_0^2 + \xi_0^2} \right) + K_0 \left( \sqrt{\xi_0^2 + \xi_0^2} \right),
\]

(2.5)

\[
\frac{\partial T}{\partial \xi_0} = -e^{-\xi_0} \left\{ \frac{\xi_0}{\sqrt{\xi_0^2 + \xi_0^2}} \right\} K_1 \left( \sqrt{\xi_0^2 + \xi_0^2} \right),
\]

(2.6)

\[
\left| \nabla T \right| = \sqrt{\left( \frac{\partial T}{\partial \xi_0} \right)^2 + \left( \frac{\partial T}{\partial \xi_0} \right)^2}.
\]

(2.7)

In equation (2.4), the variable \(\tau\) is related to the variable \(\xi_0\) as \(\xi_0 = \tau - 1\), where \(\tau\) is defined as \(\tau = \frac{t}{\rho c V^2}\). Also in equations (2.4), (2.5) and (2.6), \(K_1\) is the modified Bessel function of the second kind and order 1.

The relationship between dimensionless cooling rate \(\left( \frac{\partial T}{\partial \tau} \right)\) and actual cooling rate \(\left( \frac{\partial T}{\partial t} \right)\) and that between dimensionless thermal gradient \(\left| \nabla T \right|\) and actual thermal gradient \(\left| \nabla T \right|\) can be expressed as

\[
\frac{\partial T}{\partial \tau} = \left( \frac{2\pi k^2 b}{\alpha Q p c V^2} \right) \frac{\partial T}{\partial t}, \quad \left| \nabla T \right| = \left( \frac{2\pi k^2 b}{\alpha Q p c V} \right) \left| \nabla T \right|.
\]

(2.8)

Values of the dimensionless cooling rate and thermal gradient at the onset of solidification are obtained by evaluating the equations (2.4) and (2.7) along the boundary of the melt pool. The coordinates \((x_0, z_0)\) which lie on the boundary of the melt pool are obtained by replacing \(T\) with
the melting point $T_m$ and finding the roots of equation (2.2) numerically. The numerical root finding was conducted using the software package MATLAB, and results for melt pool length were verified against those previously published in the literature [18, 48, 51].

In conjunction with the dimensionless variables defined in equations (2.3), (2.4), (2.7) and (2.8), the Rosenthal solution enables the development of process maps for cooling rate and thermal gradient throughout the depth of the melt pool. Such results are shown in Figures 2.3 and 2.4, where the dimensionless cooling rate and thermal gradient are plotted as a function of normalized melting temperature $\overline{T}_m$ and relative depth within the melt pool $\overline{z_m}$. The normalized melting temperature varies with laser power, and is defined in terms of the melting temperature $T_m$ as

$$\overline{T}_m = \frac{T_m - T_0}{\alpha Q \pi k b}.$$  \hfill (2.9)

The normalized depth varies in the range $0 \leq \overline{z_m} \leq 1$, where $\overline{z_m}$ signifies the deepest extent of the melt pool for a given value of $\overline{T}_m$.

![Figure 2.3: Cooling Rate Process Map for Thin-Wall Geometries](image)

Figure 2.3: Cooling Rate Process Map for Thin-Wall Geometries
Figure 2.4: Thermal Gradient Process Map for Thin-Wall Geometries

The results of Figures (2.3) and (2.4) indicate that for fixed material properties, changes in laser power (or changes in $T_m$) can have a significant effect on the dimensionless cooling rate and thermal gradient, and hence the resulting microstructure. When plotted on a log scale (not shown here), the results indicate that changes in laser power can change both the dimensionless cooling rate and thermal gradient by several orders of magnitude. The cooling rate process map (Figure 2.3) reveals a significant variance of the cooling rate through the depth of the melt pool for a given laser power and velocity, especially for high values of $T_m$. Cooling rate decreases with depth within the melt pool, with a maximum value at the surface and a minimum value at the bottom of the melt pool. In contrast, the process map for thermal gradient (Figure 2.4) reveals that the thermal gradient is insensitive to depth for a given laser power and velocity. It should be noted that thermal gradient increases slightly with depth within the melt pool. However, this variance of thermal gradient through the depth of melt pool is small when compared to the variance of the cooling rate, and therefore is not clearly noticeable on the plot. This supports the conclusion that thermal gradient is relatively insensitive to depth. Moreover, increasing laser power (or decreasing $T_m$) results in a substantial decrease in thermal gradient at all depths within the melt pool, while the cooling rate for the same comparison is most significantly affected at the surface. Hence, increasing laser power
(i.e., increasing process size scale) acts to decrease the high thermal gradients typically associated with a columnar microstructure, with an increase in solidification rate (ratio of cooling rate to thermal gradient) towards the surface of the deposit. This suggests the potential for a grading of the microstructure throughout the depth of the deposit, with a transition from columnar to equiaxed microstructure at the surface.

In 2-D, the only effect of laser velocity on either cooling rate or thermal gradient is through the normalizations of equation (2.8). For fixed values of $T_m$ (or fixed laser power), changes in laser velocity affect cooling rate and thermal gradient only through the normalizations of equation (2.8). Inspection of equation (2.8) reveals that the cooling rate is more sensitive to laser velocity than thermal gradient, as the former scales with the square of the velocity while the latter scales linearly with the laser velocity. Still, changes in laser velocity can also have a significant effect on both solidification cooling rate and thermal gradient. Finally, both the thermal gradient and solidification velocity (the ratio of cooling rate to thermal gradient) scale linearly with laser velocity, which depending upon the material system might also influence trends in grain morphology.

### 2.3 Process Map Development for Bulky 3-D Geometries

The Rosenthal point source solution for three-dimensional flow of heat in a semi-infinite solid (Figure 2.2) is given as [60]

$$T - T_0 = \frac{\alpha Q}{2\pi k} e^{-\lambda Vx_0} e^{-\lambda VR} \frac{e^{-\lambda VR}}{R}. \tag{2.10}$$

With the exception of $R$, the definitions of all the terms in equation (2.10) are same as those in equation (2.1). In equation (2.10), $R = \sqrt{x_0^2 + y_0^2 + z_0^2}$ is the radial distance from the point heat source.

The Rosenthal 3-D solution of equation (2.10) can be expressed in dimensionless form as [50] [49] [18].

$$\mathcal{T} = e^{-\left(x_0^{\frac{1}{2}} + y_0^{\frac{1}{2}} + z_0^{\frac{1}{2}}\right)} \frac{e^{-\lambda VR}}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}, \tag{2.11}$$

Where
\[ \bar{T} = \frac{T - T_0}{\left(\frac{\alpha Q}{\pi k}\right)^{1/2}}, \quad \bar{x}_0 = \frac{x_0}{\sqrt{\pi}}, \quad \bar{y}_0 = \frac{y_0}{2k/pcV}, \quad \text{and} \quad \bar{z}_0 = \frac{z_0}{2k/pcV}. \]  

(2.12)

The above definition of \( \bar{T} \) is in keeping with that used for bulky 3-D geometries in [18,49,50,61], and differs by a factor of 2 from a more recent definition used by other researchers [100–102].

Comparisons of equations (2.12) and (2.3) reveals that in terms of the laser deposition process variables, the temperature normalization of bulky 3-D geometries is different from that for thin-wall geometries. The 2-D normalization is only a function of laser power, while the 3-D normalization depends upon both laser power and velocity. However, the spacial normalizations of \( \bar{x}_0, \bar{y}_0 \) and \( \bar{z}_0 \) are the same for both 2-D and 3-D geometries. The dimensionless cooling rate and thermal gradient for 3-D geometries can be obtained by differentiating equation (2.11). The expression for dimensionless cooling rate is given by equation (2.13) and that of dimensionless thermal gradient is given by equation (2.17).

\[ \frac{\partial \bar{T}}{\partial t} = \frac{1}{2} e^{-\left\{ \frac{\left(\tau - \tau_0 + \sqrt{\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2} \right)}{\sqrt{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)}} \right\}} \left\{ 1 - \frac{\left(\tau - \tau_0\right)}{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} + \frac{\left(\tau - \tau_0\right)}{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} \right\}, \]  

(2.13)

\[ \frac{\partial \bar{T}}{\partial \bar{x}_0} = \frac{1}{2} e^{-\left\{ \frac{\left(\tau + \sqrt{\tau^2 + \bar{y}_0^2 + \bar{z}_0^2}\right)}{\sqrt{\tau^2 + \bar{y}_0^2 + \bar{z}_0^2}} \right\}} \left\{ 1 - \frac{\bar{x}_0}{\left(\bar{x}_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} + \frac{\bar{x}_0}{\left(\bar{x}_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} \right\}, \]  

(2.14)

\[ \frac{\partial \bar{T}}{\partial \bar{y}_0} = -\frac{1}{2} e^{-\left\{ \frac{\left(\tau_0 + \sqrt{\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2}\right)}{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} \right\}} \left\{ 1 + \frac{1}{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} \right\}, \]  

(2.15)

\[ \frac{\partial \bar{T}}{\partial \bar{z}_0} = -\frac{1}{2} e^{-\left\{ \frac{\left(\tau_0 + \sqrt{\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2}\right)}{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} \right\}} \left\{ 1 + \frac{1}{\left(\tau_0^2 + \bar{y}_0^2 + \bar{z}_0^2\right)} \right\}, \]  

(2.16)

\[ |\nabla \bar{T}| = \sqrt{\left(\frac{\partial \bar{T}}{\partial \bar{x}_0}\right)^2 + \left(\frac{\partial \bar{T}}{\partial \bar{y}_0}\right)^2 + \left(\frac{\partial \bar{T}}{\partial \bar{z}_0}\right)^2}. \]  

(2.17)
In equation (2.13), the variable \( \bar{x} \) is related to the variable \( \bar{x}_0 = \bar{x} - \bar{t} \), where \( \bar{t} \) is defined as
\[
\bar{t} = \frac{t}{pcV^2}.
\]

The relationship between dimensionless cooling rate \( \left( \frac{\partial T}{\partial \bar{t}} \right) \) and actual cooling rate \( \left( \frac{\partial T}{\partial t} \right) \) and that between dimensionless thermal gradient \( \left( |\nabla T| \right) \) and actual thermal gradient \( \left( |\nabla T| \right) \) can be expressed as
\[
\frac{\partial T}{\partial \bar{t}} = \left( \frac{2k}{pcV} \right)^2 \left( \frac{\pi k}{\alpha QV} \right) \frac{\partial T}{\partial t}, \quad |\nabla T| = \left( \frac{2k}{pcV} \right)^2 \left( \frac{\pi k}{\alpha Q} \right) |\nabla T| . \tag{2.18}
\]

Equation (2.18) reveals that the 3-D definitions of dimensionless cooling rate and thermal gradient have a higher order velocity dependence compared to the 2-D normalizations of equation (2.8), which is a direct result of the temperature normalization of equation (2.12).

Analogous to the procedures followed for thin-wall geometries, values of the dimensionless cooling rate and thermal gradient at the onset of solidification for bulky 3-D geometries are obtained by evaluating the equations (2.13) and (2.17) along the boundary of the melt pool cross section in the \((x,z)\) plane (i.e., along \( \bar{x}_0 = 0 \)). The resulting process maps for solidification cooling rate and thermal gradient are plotted in Figs. 2.5 and 2.6 as a function of normalized melting temperature \( \bar{T}_m \) and relative depth within the melt pool \( \bar{z}_m \). Note that according to eq. (2.12), the dimensionless melting temperature for bulky 3-D geometries is defined in terms of both laser power and velocity as
\[
\bar{T}_m = \frac{T_m - T_0}{\left( \frac{\alpha Q}{\pi k} \right) \left( \frac{pcV}{2k} \right)} . \tag{2.19}
\]
The results of Figures. 2.5 and 2.6 indicate that for fixed material properties, changes in laser power or velocity (or changes in $T_m$) can have a significant effect on cooling rate and thermal gradient, and hence the resulting microstructure. When plotted on a log scale (not shown here), the
results indicate that changes in laser power or velocity can change both the dimensionless cooling rate and thermal gradient by several orders of magnitude. The results of Figs. 2.5 and 2.6 reveal that for a fixed laser velocity, trends in dimensionless cooling rate and thermal gradient are similar to those observed for thin-wall geometries in Figs. 2.3 and 2.4. However, the dimensionless thermal gradient in 3-D is slightly more sensitive to depth within the deposit, especially at the bottom of the melt pool, and the dimensionless cooling rate in 3-D shows significant variation throughout the depth of the melt pool for almost all values of $T_m$. Also, owing to the different temperature normalizations in 2-D and 3-D, comparing the magnitudes of the dimensionless results in Figs. 2.3, 2.4 with those of Figs. 2.5 and 2.6 can be misleading. For example, although the magnitudes of the dimensionless cooling rates are larger in Fig. 2.3 than in Fig. 2.5, the actual cooling rate for a given laser power and velocity is greater in 3-D than in 2-D. Further in contrast to 2-D, the variations in laser velocity affects the value of $T_m$ for 3-D geometries, which complicates the interpretation of the axes in Figs. 2.5 and 2.6. However, if it is assumed that the velocity is held constant, all previous conclusions regarding the effect of laser power (i.e., process size scale) on grain morphology are applicable to bulky 3-D deposits as well.

The actual cooling rate and thermal gradient in 3-D (eq. 2.18) are more sensitive to laser velocity, as compared to their counterparts in 2-D (eq. 2.8). The actual cooling rate in 3-D scales with the cube of the laser velocity, whereas the thermal gradient scales with the square of the velocity. However, in similarity to 2-D, the solidification velocity (ratio of cooling rate to thermal gradient) in 3-D scales linearly with laser velocity. Therefore, depending on the material system considered, laser velocity can potentially influence trends in grain morphology.

An important point to note is that the range of laser velocities considered both in small-scale deposition of thin-wall geometries and in the small and large-scale deposition of bulky structures is comparable (on the order of 5-25 inches/minute). However at the same time the range of laser powers can span as much as two orders of magnitude (300-30,000 W). Therefore, most of the discussion in this dissertation on the effects of process scaling will focus primarily on laser power.
2.4 Solidification Maps for Predicting Grain Morphology in Laser-Deposited Ti-6Al-4V

This section presents solidification map predictions for the Ti-6Al-4V material system based on the solidification cooling rate and thermal gradient process maps previously discussed. An important point to reiterate here is that, the Rosenthal results neglect the nonlinear effects of temperature-dependent properties and latent heat of transformation. In the next chapter, thermal finite element analysis will be presented that will include the nonlinear effects neglected by the Rosenthal solution, and thereby assess the utility of the Rosenthal solution for predicting trends in solidification microstructure.

As discussed in [53,55,56,58,61,62], results for solidification thermal gradient and cooling rate can be interpreted in the context of a solidification map to provide predictions of grain morphology in laser-deposited Ti-6Al-4V. Given the solidification cooling rate $\frac{\partial T}{\partial t}$ and thermal gradient $G = |\nabla T|$, the solidification velocity $R$ is determined as

$$R = \frac{1}{G} \frac{\partial T}{\partial t}, \quad (2.20)$$

The expected grain morphology can be predicted as either equiaxed, columnar or mixed by plotting points in $G$ vs. $R$ space (i.e., on the "solidification map"), which has been previously calibrated for Ti-6Al-4V [53,55,58].

2.4.1 Solidification Map Predictions for Thin-Walled Geometries

Solidification maps showing the effects of laser power and velocity for small-scale (LENS™) deposition of thin-wall geometries are shown in Figs. 2.7 and 2.8. The range of laser powers and velocities considered are typical of those used in the LENS™ deposition of thin-wall geometries. The results of Figs. 2.7 and 2.8 are extracted directly from the Rosenthal results of Figs. 2.3 and 2.4, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ C$. The Rosenthal results assume the fraction of the absorbed laser power to be $\alpha = 0.35$, which has been previously calibrated for LENS™ deposition of thin-wall Ti-6Al-4V deposits [17], and is very close to the value reported by Kummailil et al. [113]. The solid and dashed lines in
Figs. 2.7 and 2.8 bound the regions of fully equiaxed, fully columnar and mixed morphologies, as previously calibrated for Ti-6Al-4V [53, 55, 58].

The effect of laser power on grain morphology for a fixed laser velocity is illustrated in Fig. 2.7. The range of laser powers considered spans 150-550 W, while the laser velocity is held constant at 8.47 mm/s. From Fig. 2.7 it is clear that the data points for all powers and depths fall in the fully columnar region. This result is in keeping with both Cellular Automaton Solidification Modeling results [17] and experimental observations for LENS\textsuperscript{TM} deposited Ti-6Al-4V [17, 59]. The results of Fig. 2.7 suggest that increasing laser power at a fixed velocity (i.e., increasing laser incident energy) tends to shift the data towards the boundary of fully columnar/mixed morphology.

![Graph](image)  

**Figure 2.7:** Predicted Ti-6Al-4V Grain Morphology for Small-Scale (LENS\textsuperscript{TM}) Deposition of Thin-Wall Deposits from 2-D Rosenthal Solution (Effect of Laser Power)

The effect of laser velocity on grain morphology at a fixed laser power is illustrated in Fig. 2.8. The range of laser velocities considered spans 2.12-10.6 mm/s, while the laser power is held constant at $Q = 350$ W. In Fig. 2.8, the data points for all velocities and depths fall in the fully columnar region, which is again in keeping with both Cellular Automaton Solidification Modeling results [17] and experimental results observations for LENS\textsuperscript{TM} deposited Ti-6Al-4V [17, 59]. Results of Fig. 2.8 suggest that decreasing the laser velocity at a fixed power (increasing the laser incident energy)
would tend to shift the data towards the boundary of fully columnar/mixed morphology.

Figure 2.8: Predicted Ti-6Al-4V Grain Morphology for Small-Scale (LENS\textsuperscript{TM}) Deposition of Thin-Wall Deposits from 2-D Rosenthal Solution (Effect of Laser Velocity)

\section*{2.4.2 Solidification Map Predictions for Small-Scale (LENS\textsuperscript{TM}) Deposition of Bulky Geometries}

Solidification maps showing the effects of laser power and velocity for small-scale (LENS\textsuperscript{TM}) deposition of bulky geometries are shown in Figs. 2.9 and 2.10. The range of laser powers and velocities considered are typical of that used in the LENS\textsuperscript{TM} deposition of bulky geometries. The results of Figs. 2.9 and 2.10 are extracted directly from the Rosenthal results of Figs. 2.5 and 2.6, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654\,^{\circ}C$. Again, as in the previous section the Rosenthal results assume the fraction of the absorbed laser power to be $\alpha = 0.35$.

The effect of laser power on grain morphology at constant velocity is presented in Fig. 2.9. The range of laser powers is 350-850 W, which is larger than that considered for thin-wall geometries presented in the previous section. However the laser velocity is held constant at $8.47\, mm/s$, the same value used in the thin-wall analysis. From Fig. 2.9, it is clear that the Rosenthal results predict fully
columnar morphology, which is in keeping with experimental observations for LENSTM deposition of bulky Ti-6Al-4V structures [53–55, 58] and recent Cellular Automaton Solidification Modeling results [107]. Further, the results also suggest that increasing laser power tends to shift the data closer to the boundary for fully columnar/mixed morphology. These results are in keeping with G vs. R predictions reported for thin-wall geometries in the previous section.

![Small-Scale (LENSTM); 3-D Rosenthal Effect of Laser Power (V = 8.47 mm/s)](image)

Figure 2.9: Predicted Ti-6Al-4V Grain Morphology for Small-Scale (LENSTM) Deposition of Bulky 3-D Deposits from 3-D Rosenthal Solution (Effect of Laser Power)

The effect of laser velocity on grain morphology at a fixed laser power is illustrated in Fig.2.10. Here, the range of laser velocities considered are the same as that for thin-wall analysis (2.12-10.6 mm/s), while the laser power is held constant at $Q = 550 W$. Results of Fig. 2.10 predict fully columnar morphology, which is in keeping with experimental observations [53–55, 58] and recent Cellular Automaton Solidification Modeling results [107]. However a decrease in laser velocity, at a fixed power (i.e increasing laser incident energy) shifts the trends towards the fully columnar/mixed boundary. This supports the results reported previously for 2-D thin-wall geometries.
Figure 2.10: Predicted Ti-6Al-4V Grain Morphology for Small-Scale (LENS™) Deposition of Bulky 3-D Deposits from 3-D Rosenthal Solution (Effect of Laser Velocity)

2.4.3 Solidification Map Predictions for Large-Scale Deposition of Bulky Geometries

Solidification maps showing the effects of laser power and velocity for large-scale (higher power) deposition of Ti-6Al-4V bulky geometries are shown in Figs. 2.11 and 2.12. The results of Figs. 2.11 and 2.12 are extracted directly from the Rosenthal results of Figs. 2.5 and 2.6, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654°C$. Again, the Rosenthal results assume the fraction of the absorbed laser power to be $\alpha = 0.35$.

Figure. 2.11 reveals the effect of laser power on grain morphology at a fixed laser velocity. The range of laser powers considered spans $5 – 30kW$, while the laser velocity is held constant at $V = 8.47mm/s$. Results of Fig. 2.11 suggest that large-scale processes can result in a grading of microstructure throughout the depth of the deposit, with a mixed or even fully equiaxed microstructure at the surface. Moreover, the trend towards equiaxed microstructure increasing with laser power (increasing incident energy) is clearly illustrated in Fig. 2.11. Experimental results reported in the literature [58] and recent Cellular Automaton Solidification Modeling results [107], support this

37
columnar to equiaxed transition at high powers predicted by the solidification map. The results presented in [58] are for a 14 kW large-scale process.

These above trends can be inferred from the discussion of thermal process maps of Figs. 2.3, 2.4, 2.5 and 2.6. In particular, increasing laser power (i.e., size-scale) acts to reduce thermal gradients, which for a fixed cooling rate would move the data down and to the right in the G vs. R space. However, at the same time increases power also decreases cooling rates (and hence the solidification rate R), which is a competing effect. The net result is essentially downward movement in G vs. R space. Therefore, the trend towards mixed or equiaxed microstructure at the surface increases with an increase in laser power (size-scale).

Figure 2.11: Predicted Ti-6Al-4V Grain Morphology for Large-Scale (High-Power) Deposition of Bulky 3-D Deposits from 3-D Rosenthal Solution (Effect of Laser Power)

Figure. 2.12 reveals the effect of laser velocity on grain morphology at a fixed laser power. The range of laser velocities considered spans 2.12-10.6 mm/s, while the laser power is held constant at \( Q = 15000 \text{W} \). It is important to note that the range of laser velocities considered for large-scale processes is similar to that considered during small-scale analysis of thin-wall and bulky geometries. This is because as said previously, the velocities used in small-scale and large-scale processes are comparable. The Results of Fig. 2.12 suggest that large-scale processes can result in a grading
of microstructure throughout the depth of the deposit, with a mixed or even fully equiaxed microstructure at the surface in agreement with recent Cellular Automaton Solidification Modeling results [107]. Again, these trends can be inferred from the discussion of thermal process maps of Figs. 2.3, 2.4, 2.5 and 2.6. In particular, decreasing laser velocity at a fixed power acts to decrease thermal gradients, which for a fixed cooling rate would move the data down and to the right in the G vs. R space (analogous to increasing laser power). However, at the same time decreasing velocity also decreases cooling rates (and hence the solidification rate R), which is a competing effect. The net result is essentially downward movement in G vs. R space

![Graph](https://via.placeholder.com/150)

Figure 2.12: Predicted Ti-6Al-4V Grain Morphology for Large-Scale (High-Power) Deposition of Bulky 3-D Deposits from 3-D Rosenthal Solution (Effect of Laser Velocity)

### 2.5 Chapter Summary

In this chapter, thermal process maps for solidification cooling rates and thermal gradients, have been developed based on the well known Rosenthal solution for a moving point heat source traversing an infinite substrate. Process maps have been developed for both 2-D thin-walled and 3-D bulky deposits. These process maps are applicable to any material system. Finally, the results of these process maps are interpreted in the context of a solidification map, for predicting trends in grain
morphology in the Ti-6Al-4V material system.
3 Inclusion of Nonlinearity Through
Thermal Finite Element Analysis

In this dissertation, the primary purpose of the finite element modeling is to assess the validity of the Rosenthal solution for predicting trends in solidification microstructure by including the nonlinear effects of temperature-dependent properties and latent heat. Thermal finite element analysis is carried out to model

- The deposition of thin-walled Ti-6Al-4V geometries for the small-scale (LENS™) process
- The deposition of bulky 3-D Ti-6Al-4V geometries for both small-scale (LENS™) and large-scale (high power) processes.

Continuum finite element modeling of laser deposition processes is fairly well established and has been successfully used to study the effects of process variables on melt-pool size and residual stress [18, 48–51]. The thermal finite element modeling procedures adopted in this dissertation are analogous to those used by Vasinonta et. al., [18, 48–51] in studies of melt-pool size and residual stress in laser deposition of thin-wall and bulky stainless steel structures.

3.1 2-D Thermal Finite Element Modeling

In this section, the thin-walled geometry of Fig. 2.1 is considered. The chosen geometry is representative of thin-wall structures commonly built using the LENS™ and other small-scale laser deposition processes. Here, the wall thickness \( b \) is assumed to be much less than the length \( L \) and height \( h \), so that heat conduction is restricted to the \((x,z)\) plane. Moreover, it is assumed that the length \( L \) and height \( h \) are sufficiently large such that the steady-state 2-D Rosenthal solution for a point heat source traversing an infinite half-space applies.
The thermal Finite Element (FE) models used in this study consider only the problem of heat conduction within the melt pool and the surrounding thin-wall geometry, with all free surfaces assumed to be insulated. Thus the FE models used here, do not include the effects of

- Radiation from the surface of the melt pool
- Convective heat transfer between the free surfaces of the wall and the surrounding air
- Convective flows within the melt pool
- Evaporation of the molten metal

Dobranich and Dykhuizen [73, 76] suggested in their work that these other modes of heat transfer (convection, radiation and evaporation) are generally small compared to conduction in laser deposition processes and hence their effects can be neglected. In the thermal finite element models presented here, the laser is modeled as moving point heat source, so that the actual distribution of power is neglected. Such an assumption is most appropriate for cases in which the melt pool is sufficiently large relative to the laser beam width, and has been previously found to provide reasonable predictions of melt pool size in thin-wall LENS™ deposits [18,51]. This also allows for the validation of the 2-D Rosenthal solution that was used for predicting trends in solidification microstructure in the previous chapter. Finally, the thermal finite element models do not explicitly include material addition (i.e., the powder feed rate) during the laser pass. While the effect of material addition can be grossly approximated through the fraction of the absorbed laser power $\alpha$, the current modeling approach is most strictly applicable for a single laser pass across an existing thin-wall.

The finite element modeling was carried out using the commercial software package ABAQUS. A representative 2-D thermal finite element mesh and boundary conditions for the thin-wall geometry of Fig. 2.1 is illustrated in Fig. 3.1. The model uses 4-noded bi-linear thermal elements as part of the ABAQUS software package.

The finite element model approximates the laser deposition process as a moving point heat source $\alpha Q$, which is successively applied to adjacent nodes (beginning at the left end) at time intervals corresponding to the laser velocity $V$. The parameter $\alpha$ represents the fraction of the laser power absorbed by the deposit, and based on previous results in the literature has been estimated as 35% [17,18,51,113]. This value gives reasonable agreement with melt pool sizes observed for the
Figure 3.1: Representative 2-D Thermal Finite Element Mesh

LENS™ process [17]. The remaining boundary conditions are approximated as insulated \((q = 0)\) on the top and both vertical edges, with a fixed temperature condition on the bottom \((T = 25 \, ^\circ C)\). As discussed by Vasinonta et. al., [18, 51], the presence of natural convection on the edges is essentially equivalent to thermal insulation. While the fixed room temperature condition on the bottom neglects any inherent preheating of the base during material deposition, its effect on thermal gradient and cooling rate in close proximity to the laser (i.e., within the melt pool) is assumed to be small. Finally, the finite element model uses temperature-dependent specific heat, density and thermal conductivity, and includes latent heat effects for Ti-6Al-4V.

A representative contour plot illustrating the transient temperature distribution is shown in Fig. 3.2 for the case of \(Q = 350 \, W\) and \(V = 8.47 \, mm/s\). In Figure 3.2, the location of the laser is evident from the intensity of the temperature distribution, where the maximum contour limit of 1650 \(^\circ C\) signifies the melt pool. As shown in the Figure, the thermal history is essentially independent of the vertical free edges once the laser has reached the center of the wall, where the mesh has been highly refined (Fig.3.1) for accurate extraction of the thermal gradient and cooling rate. In general, the mesh resolution of Fig. 3.1 has provided more than 10 elements through the depth of the melt pool, so that both thermal gradient and cooling rate at the onset of solidification can be determined as a function of vertical location beneath the surface.
3.2 Extraction of Cooling Rate and Thermal Gradient

The cooling rate and thermal gradient at the onset of solidification have been extracted from the 2-D model results at various nodal locations throughout the depth of the melt pool. At each nodal location the solidification cooling rate is determined as

\[
\frac{\partial T}{\partial t} = \frac{|T_S - T_L|}{t_S - t_L}.
\]  

In equation (3.1), \( T_L \) and \( T_S \) are the liquidus and solidus temperatures reached at times \( t_L \) and \( t_S \) respectively. As defined in equation (3.1), the cooling rate is an average value taken throughout the time required for solidification. The thermal gradient evaluated at the time \( t = t_L \) is determined directly from the nodal heat flux output, and is obtained from Fourier’s law as

\[
G = |\nabla T| = \frac{|\vec{q}|}{k}.
\]

In equation (3.2), \( |\vec{q}| \) is the magnitude of the heat flux vector and \( k \) is the thermal conductivity at the liquidus temperature. Finally, the solidification cooling rate and thermal gradient determine the solidification velocity \( R \) as

\[
R = \frac{1}{G} \frac{\partial T}{\partial t}.
\]

Following the calculation of \( G \) and \( R \), the expected grain morphology can be calculated as ei-
ther equiaxed, columnar or mixed by plotting points in G vs. R space (i.e., on the "solidification map") [53, 55, 58]. In the next section, a comparison between 2-D FEM and 2-D Rosenthal results will be interpreted in the context of solidification map to predict the effects of laser power and velocity on grain morphology in the Ti-6Al-4V material system. The basic idea of the comparison as said previously is to assess the utility of the Rosenthal solution (which neglects nonlinear effects of temperature-independent properties and latent heat) for predicting trends in solidification microstructure.

### 3.3 Comparison Between 2-D FEM and 2-D Rosenthal Results

Solidification maps showing the effects of laser power and velocity over a range of typical LENS\(^\text{TM}\) process variables for thin-wall Ti-6Al-4V deposits are shown in Figures 3.3 and 3.4. The results of Figs. 3.3 (a) and 3.4 (a) have been extracted from 2-D thermal FEM analyses of the thin-wall geometry of Fig. 2.1. The FEM results include temperature-dependent properties and latent heat effects for Ti-6Al-4V. The results of Figs. 3.3 (b) and 3.4 (b) are extracted directly from the Rosenthal results of Figs. 2.3 and 2.4, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature \(T_m = 1654^\circ C\). The difference between the Rosenthal results presented here and that presented in the previous chapter is that here the Rosenthal results are presented at approximately the same nodal locations as in the FEM. Both the FEM and Rosenthal results assume the fraction of the absorbed laser power to be \(\alpha = 0.35\).

Although the Rosenthal results neglect the nonlinear effects of temperature-dependent properties and latent heat of transformation, trends in G vs. R data are in reasonably good agreement with the FEM results. In particular, both the Rosenthal and FEM results predict a fully columnar morphology, which is in keeping with Cellular Automaton Solidification Modeling results [17] and experimental observations of LENS\(^\text{TM}\) deposited Ti-6Al-4V [17, 59]. However, results also suggest that increasing laser incident energy (increasing power or decreasing velocity) tends to shift the data closer to the boundary of fully columnar/mixed morphology. This is in agreement with the conclusions presented earlier based solely on the Rosenthal solution.
Small-Scale (LENS\textsuperscript{TM}): 2-D FEM
Effect of Laser Power (V = 8.47 mm/s)

\(Q = 315\) W
\(Q = 350\) W
\(Q = 385\) W

(a) 2-D FEM

Small-Scale (LENS\textsuperscript{TM}): 2-D Rosenthal
Effect of Laser Power (V = 8.47 mm/s)

Increasing \(Z\) (Depth)

(b) 2-D Rosenthal

Figure 3.3: Predicted Grain Morphology for Small-Scale (LENS\textsuperscript{TM}) Deposition of Thin-Walled Geometries from (a) 2-D FEM and (b) 2-D Rosenthal (Effect of Laser Power)
Figure 3.4: Predicted Grain Morphology for Small-Scale (LENS\textsuperscript{TM}) Deposition of Thin-Walled Geometries from (a) 2-D FEM and (b) 2-D Rosenthal (Effect of Laser Velocity)
3.4 3-D Thermal Finite Element Modeling

In this section the geometry of Fig. 2.2 is considered. Here again, as with the thin-walled structures, the dimensions of the geometry are assumed to be large enough such that the steady-state 3-D Rosenthal solution for a point heat source traversing an infinite half-space applies. Also, taking advantage of the symmetry, only a half-model is considered for the analysis. Similar to the thin-walled simulations, the numerical models used here do not include the effects of radiation from the surface of the melt pool, convective heat transfer between the wall free surfaces and the surrounding air, convective flows within the melt pool and evaporation of the molten metal. Here again, as in the case of 2-D models, the laser is modeled as a moving point heat source. This allows for the validation of the 3-D Rosenthal solution that was used for predicting trends in solidification microstructure in the previous chapter.

A representative finite element mesh and boundary conditions for a half-symmetric model of a bulky 3-D geometry is shown in Fig. 3.5. The model uses 8-noded bi-linear thermal elements, and has been generated using the software package ABAQUS. As said previously, the finite element model approximates the laser deposition process as a moving point heat source $\alpha Q$, which is successively applied to adjacent nodes at time intervals corresponding to laser velocity $V$. As in the 2-D simulations, the parameter $\alpha$ represents the fraction of the absorbed laser power, and has been estimated as 0.35 %. The boundary conditions imposed are insulation ($q = 0$) on the top and all side faces, and a fixed temperature condition at the bottom ($T = 25^\circ C$). Finally, the finite element model uses temperature-dependent specific heat, density and thermal conductivity, and also includes latent heat effects for Ti-6Al-4V.
Meshes similar to that of Fig. 3.5 have been used to investigate small-scale deposition of bulky geometries. When investigating the large-scale deposition of bulky geometries, the mesh of Fig. 3.5 was scaled in all the three dimensions. For each of the various powers considered during investigation of the large-scale deposition of bulky geometries, the dimensions of the mesh have been scaled such that the behavior in the vicinity of the melt pool is unaffected by the boundaries. This is in keeping with the steady-state Rosenthal solution. In general, the mesh resolution of Fig. 3.5 has provided more than 10 elements through the depth of the melt pool, from which solidification cooling rates and thermal gradients have been extracted. Procedures for extracting solidification cooling rates and thermal gradients from the finite element results follow those outlined previously during the discussion of thin-wall geometries and are not reiterated here.

A rigorous convergence study in both space and time is carried out for the case of temperature-independent properties, so that the numerical results (of cooling rates and thermal gradients) could be directly compared with the analytical results obtained using the Rosenthal solution. The spatial convergence study was carried out by increasing the mesh resolution by a factor of 2 in the $x$, $y$ and $z$ directions as we move from coarse to medium and then to fine meshes. The coarse, medium and fine meshes used for the convergence study are shown in Fig. 3.6 (a), (b) and (c) respectively. Convergence studies in time were carried out by increasing the time increments by a factor of 2.
The finite element results for both cooling rate and thermal gradient showed clear convergence in both space and time as we move from coarse to medium and then to fine. The FEM convergence study also recovered solidification cooling rates and thermal gradients within two percent of the analytical Rosenthal results presented in chapter 2 of this dissertation, which clearly verifies the accuracy of the finite element modeling procedures. The convergence study was carried out at three nodes, which are present at the same location in the coarse, medium and fine meshes. The results of the convergence study are presented for two nodes in Figs. 3.7, 3.8, 3.9 and 3.10. Figures 3.7 (a) and 3.8 (a) illustrate the convergence of cooling rate at the two different nodes in space, whereas Figs. 3.7 (b) and 3.8 (b) illustrate the convergence of cooling rate in time. Similarly, Figs. 3.9 (a) and 3.10 (a) illustrate the convergence of thermal gradient at the two different nodes in space, while the Figs. 3.9 (b) and 3.10 (b) illustrate the convergence of thermal gradient in time.
Figure 3.6: Coarse (a), Medium (b) and Fine (c) Meshes Used in the Convergent Study
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Figure 3.7: Convergence of Cooling Rate at Node1 in (a) Space and (b) Time

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(b) Time

Figure 3.8: Convergence of Cooling Rate at Node2 in (a) Space and (b) Time

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(b) Time

Figure 3.9: Convergence of Thermal Gradient at Node 1 in (a) Space and (b) Time
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</table>

(b) Time

Figure 3.10: Convergence of Thermal Gradient at Node 2 in (a) Space and (b) Time
3.4.1 Comparison Between 3-D FEM and 3-D Rosenthal Results for Small-Scale (LENS™) Deposition of Bulky Deposits

Solidification maps showing the effects of laser power and velocity for small-scale (LENS™) deposition of bulky geometries are shown in Figs. 3.11 and 3.12. The range of laser powers and velocities considered are typical of that used in the LENS™ deposition of bulky geometries. The results of Figs. 3.11 (a) and 3.12 (a) are extracted using the 3-D finite element mesh shown in Fig. 3.5, with temperature-dependent properties and latent heat effects for Ti–6Al-4V. While the results of Figs. 3.11 (b) and 3.12 (b) are extracted directly from the Rosenthal results of Figs. 2.5 and 2.6, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654°\text{C}$. Here again, the Rosenthal results are presented at approximately the same nodal locations as in FEM. Again, as in the previous section both the FEM and Rosenthal results assume the fraction of the absorbed laser power to be $\alpha = 0.35$.

The effect of laser power on grain morphology at a constant velocity is presented in Figs. 3.11 (a) and 3.11 (b). The range of laser powers considered is 350-850 W, which is larger than that considered for thin-wall geometries presented in the previous section. However the laser velocity is held constant at $8.47 \text{mm/s}$, the same value used in the thin-wall analysis. As observed for 2-D thin-wall geometries, trends in $G$ vs. $R$ predictions from 3-D FEM and 3-D Rosenthal are in good agreement. In particular, both the 3-D FEM and Rosenthal results predict a fully columnar morphology, which is in keeping with experimental observations for LENS™ deposition of bulky Ti-6Al-4V structures [53–55, 58] and recent Cellular Automaton Solidification Modeling results [107]. Further, both the FEM and Rosenthal results clearly suggest that increasing laser power tends to shift the data closer to the boundary for fully columnar/mixed morphology. These results are in keeping with $G$ vs. $R$ predictions reported for thin-wall geometries in the previous section.

The effect of laser velocity on grain morphology at a fixed laser power is illustrated in Figs.3.12 (a) and 3.12 (b). Here, the range of laser velocities considered are the same as that considered for thin-wall analysis (2.12-10.6 mm/s), while the laser power is held constant at $Q = 550W$. Results of Fig. 3.12 (a) and 3.12 (b) show that even though the Rosenthal results neglect the non-linear effects of temperature-dependent properties and latent heat of transformation, trends in $G$ vs. $R$ data are in reasonably good agreement with the FEM results. In particular, both the 3-D Rosenthal and
FEM results predict a fully columnar morphology, which is in keeping with experimental observations [53–55, 58] and recent Cellular Automaton Solidification Modeling results [107]. However a decrease in laser velocity, at a fixed power (i.e., increasing laser incident energy) shifts the trends towards the fully columnar/mixed boundary. This supports the results reported previously for 2-D thin-wall geometries.
Figure 3.11: Predicted Grain Morphology for Small-Scale (LENS™) Deposition of Bulky Deposits from (a) 3-D FEM and (b) 3-D Rosenthal (Effect of Laser Power)
Small-Scale (LENSTM): 3-D FEM
Effect of Laser Velocity ($Q = 550$ W)

$G$ ($K/cm$)

$R$ ($cm/s$)

(a) 3-D FEM

Figure 3.12: Predicted Grain Morphology for Small-Scale (LENSTM)Deposition of Bulky Deposits from (a) 3-D FEM and (b) 3-D Rosenthal (Effect of Laser Velocity)
3.4.2 Comparison Between 3-D FEM and 3-D Rosenthal Results for Large-Scale (Higher Power) Deposition of Bulky Deposits

Solidification maps showing the effects of laser power and velocity for large-scale (higher power) deposition of bulky Ti-6Al-4V geometries are shown in Figs. 3.13 and 3.14. The results of Figs. 3.13 (a) and 3.14 (a) have been extracted from 3-D thermal finite element analyses of the bulky geometry of Fig. 2.2. While the results of Figs. 3.13 (b) and 3.14 (b) are extracted directly from the Rosenthal results of Figs. 2.5 and 2.6, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ$C. Here again, both the FEM and Rosenthal results assume the fraction of the absorbed laser power to be $\alpha = 0.35$.

Figures. 3.13 (a) and 3.13 (b) reveal the effect of laser power on grain morphology at a fixed laser velocity. The range of laser powers considered spans $5 - 30\, kW$, while the laser velocity is held constant at $V = 8.47\, mm/s$. As observed for small-scale processes, here again trends in G vs. R predictions from 3-D FEM and Rosenthal results are in good agreement. In particular, results of Figs. 3.13 (a) and 3.13 (b) suggest that large-scale processes can result in a grading of microstructure throughout the depth of the deposit, with a mixed or even fully equiaxed microstructure at the surface. Moreover, the trend towards equiaxed microstructure increasing with laser power (increasing incident energy) is clearly illustrated in Figs. 3.13 (a) and 3.13 (b). Experimental results reported in the literature [58] and recent Cellular Automaton Solidification Modeling results [107], support this columnar to equiaxed transition at high powers predicted by the solidification map. The results presented in [58], are for a 14 kW large-scale process.

These above trends can be inferred from the discussion of thermal process maps of Figs. 2.3, 2.4, 2.5 and 2.6. In particular, increasing laser power (i.e., size-scale) acts to reduce thermal gradients, which for a fixed cooling rate would move the data down and to the right in the G vs. R space. However, at the same time increasing power also decreases cooling rates (and hence the solidification rate R), which is a competing effect. The net result is essentially a downward movement in the G vs. R space. Therefore, the trend towards mixed or equiaxed microstructure at the surface increases with an increase in laser power (size-scale).

Figures. 3.14 (a) and 3.14 (b) reveal the effect of velocity on grain morphology at a fixed laser power. The range of laser velocities considered spans $2.12 - 10.6\, mm/s$, while the laser power
is held constant at $Q = 15000\, \text{W}$. It is important to note that the range of laser velocities considered for large-scale processes is similar to that considered during small-scale analysis of thin-wall and bulky geometries. This is because as said previously, the velocities used in small-scale and large-scale processes are comparable. The Results of Figs. 3.14 (a) and 3.14 (b) suggest that large-scale processes can result in a grading of microstructure throughout the depth of the deposit, with a mixed or even fully equiaxed microstructure at the surface which is in agreement with recent Cellular Automaton Solidification Modeling results [107]. Again, these trends can be inferred from the discussion of thermal process maps of Figs. 2.3, 2.4, 2.5 and 2.6. In particular, decreasing laser velocity at a fixed power (increasing laser incident energy) acts to decrease thermal gradients, which for a fixed cooling rate would move the data down and to the right in the $G$ vs. $R$ space. However, at the same time decreasing velocity also decreases cooling rates (and hence the solidification rate $R$), which is a competing effect. The net result is essentially a downward movement in the $G$ vs. $R$ space.
Figure 3.13: Predicted Grain Morphology for Large-Scale (High-Power) Deposition of Bulky Deposits from (a) 3-D FEM and (b) 3-D Rosenthal (Effect of Laser Power)
Figure 3.14: Predicted Grain Morphology for Large-Scale (High-Power) Deposition of Bulky Deposits from (a) 3-D FEM and (b) 3-D Rosenthal (Effect of Laser Velocity)
3.5 Chapter Summary

In this chapter, the nonlinear effects of temperature-dependent properties and latent heat were included through thermal finite element modeling. The 2-D and 3-D thermal finite element modeling that was carried out was discussed in detail. The procedures for extracting solidification cooling rates and thermal gradients throughout the depth of the melt pool were presented. Finally, a comparison between the FEM and Rosenthal results was interpreted in the context of a solidification map for the Ti-6Al-4V material system for both small-scale (LENS™) and large-scale (higher power) processes.
4 Transient Effects Near the Free Edge

Both the thermal process maps presented in chapter 2 as well as the thermal finite element analysis that was used to validate the utility of those process maps (chapter 3), give important insights into the effects of key deposition process variables on solidification cooling rates and thermal gradients (the key parameters controlling microstructure). However, neither addresses the issue of either the transient response in the vicinity of a free edge or the effects of transient changes in process variables. Further, the process maps that have been developed to date are applicable only if steady-state conditions exist. For instance, it is not known how the solidification cooling rates and thermal gradients change in the vicinity of a free edge, or due to sudden changes in laser power or velocity.

Rangaswamy et. al., [90] observed via direct thermal imaging of the melt pool that an increase in melt pool size occurs upon approaching a free edge, without any changes in the process variables (laser power or velocity). Aggarangsi et. al., [99] developed thermo-mechanical finite element models to both understand and control the increase in melt pool size in the vicinity of a free edge. In their work, these researchers have used the steady-state process maps developed by Vasinonta et.al., [18,48–51] to find out the power reductions that are needed to maintain a consistent melt pool size when approaching a free edge. Further, they concluded that in order to control the melt pool size effectively when approaching a free edge, a power reduction needs to be initiated before the melt pool size begins to increase.

In a recent study Aggarangsi et. al., [102] have extended the steady-state process map approach developed by Vasinonta et. al., [18,48–51] to investigate the transient changes in melt-pool size due to step changes in laser power and velocity. Finally, as discussed in the literature review section, a significant amount of progress has been made in developing real time feedback control for the LENS™ process using thermal imaging techniques for a better understanding and control of the thermal behavior during fabrication [80,81,84,86].
Despite all these advances, the effects of transient changes in melt pool size on solidification cooling rates and thermal gradients (and thereby on the resulting microstructure) have not yet been addressed. The current work addresses this problem through thermal finite element analysis of both 2-D thin-wall and bulky 3-D geometries. The research on transient effects presented in this dissertation only addresses the effect of transient melt pool response in the vicinity of the free edge. Effects of transient changes in solidification cooling rates and thermal gradients due to step changes in laser power and velocity is not considered in this dissertation, and is left for future work.

4.1 Effects Near the Free Edge for 2-D Thin-Wall Geometries

4.1.1 Modeling Approach

In this section, the thin-wall geometry of Fig. 2.1 is considered. The assumptions and the modeling approach are analogous to the ones presented in section 3.1, and hence will not be presented here. However, there is a difference in mesh density between the finite element models presented here and those presented earlier in chapter 3. The finite element models presented here have a higher mesh density near the right free edge (Fig. 4.1). This is done to facilitate the investigation of the effect of melt pool behavior in the vicinity of the free edge on solidification cooling rates and thermal gradients. The finite element model used here has three different mesh densities going from left to right (in the x-direction). A coarser mesh is used for the first sixth of the model, while the element size in the next sixth of the model is one half of the coarser region element size. Finally, the remaining portion of the model has a finer mesh where the element size is one fourth of the coarser region element size. Further, results from transient conditions are compared with results from steady-state conditions (at the center of the wall) and hence a higher mesh density is also used at the center of the wall.
In this section, thermal finite element analysis is carried out to model:

- **Case I:** The movement of the laser beginning at the left free edge of the wall, traveling left to right across the wall and reaching the right free edge. Once the laser reaches the right free edge it is turned off. Here, the effects of steady-state, transient and stationary melt pool (when the laser is turned off) behavior on solidification cooling rates and thermal gradients is investigated. Simulation results are presented for both temperature-independent and temperature-dependent (Ti-6Al-4V) properties. Results from simulations with temperature-independent properties are presented in nondimensional form, while the results from simulations with temperature-dependent properties for Ti-6Al-4V material are plotted on the solidification map of Ti-6Al-4V.

- **Case II:** The movement of the laser beginning at the left free edge of the wall, traveling left to right across the wall, reaching the right free edge and then traveling back towards the left free edge. Here, the effects of steady-state and transient melt pool behavior on solidification cooling rates and thermal gradients are investigated. In this case, only results from simulations with temperature-independent properties are presented.

Here again as in sections 2.1 and 3.1, it is assumed that the length $L$ and height $h$ are sufficiently large such that the 2-D Rosenthal solution is applicable under steady-state conditions.
4.1.2 Nondimensionalization Scheme Used for Results from Simulations with Temperature-Independent Properties

The following section describes the nondimensionalization scheme used for presenting the results from temperature-independent simulations. The nondimensionalization scheme is based on the analytical solution of Rosenthal (2-D) for a point heat source traversing a semi-infinite substrate. Since the Rosenthal solution was discussed in detail in chapter 2 of this dissertation, it will only be described here as applicable.

Based on the 2-D Rosenthal solution, a normalized melting temperature can be defined as follows (equation 2.9)

\[ T_m = \frac{T_m - T_0}{\alpha Q \pi \kappa} \]

(4.1)

Finite element simulations with temperature-independent properties are run for a representative case of the process variables: absorbed laser power \( \alpha Q = 122.5 (\alpha = 0.35, Q = 350 W) \) and laser velocity \( V = 8.47 \text{ mm/s} \), which correspond to a \( T_m = 0.96 \). Solidification cooling rates and thermal gradients are then extracted from the 2-D model at various nodal locations through the depth of the melt pool using equations 3.1 and 3.2, respectively. Upon extraction, the solidification cooling rates and thermal gradients are nondimensionalized using equation 2.8. The dimensionless cooling rates and thermal gradients are then plotted as function of relative depth within the melt pool \( \frac{z}{z_m} \). Here again the non-dimensional variable \( \frac{z}{z_m} \) is the normalized nodal distance and \( z_m \) is the deepest extent of the melt pool for a given value of \( T_m \) under steady-state conditions, as determined using the 2-D Rosenthal solution.

4.1.3 Results for Case I

This section presents the results for the case when the laser is turned off upon reaching the free edge. Here the effects of steady-state, transient and stationary melt pool behavior on solidification cooling rates and thermal gradients is presented. Figure 4.2 illustrates the increase in melt pool size as the laser approaches the free edge. An important point to note here is that the melt pool region is zoomed in Fig. 4.2 for a better view. Again as in Figure 3.2, the location of the laser (in Fig. 4.2) is evident from the intensity of the temperature distribution. As the laser moving with a constant
power and velocity reaches the center of the wall (Fig. 4.2 (a)), the melt pool size reaches a steady-state configuration. Throughout this chapter, this melt pool is referred to as steady-state melt pool. As the laser begins to approach the free edge, there is a slight increase in temperatures at all depths within the melt pool, without any noticeable change in melt pool size. Throughout this chapter, this melt pool is referred to as a transient melt pool. The size of the transient melt pool is the same as the steady-state melt pool, however the temperatures at all depths in the transient melt pool are slightly higher than the corresponding steady-state melt pool temperatures. Upon approaching the free edge, there is a considerable increase in melt pool size (Figs. 4.2 (b), (c) and (d)). This increase in melt pool size upon approaching the free edge is due to the decreased ability of the thin-wall to conduct the heat away from the melt pool.
As discussed earlier, this section considers the situation where the laser is turned off upon reaching the free edge. Throughout this chapter this melt pool is referred to as a stationary melt pool. The solidification of a stationary melt pool is illustrated in Fig. 4.3.
Values of dimensionless cooling rates and thermal gradients are plotted as a function of relative depth within the melt pool (Figs. 4.4 and 4.5) at four different x-locations in the model represented by \( \tilde{a} \). Here, \( \bar{a} \) is the normalized distance from the right free edge and \( \overline{l} \) is the steady-state melt pool length determined using the Rosenthal solution. The spacial normalization is the same as used earlier in equation 2.3. The value of \( \tilde{a} = 17.22 \) corresponds to a location at the center of the wall where the melt pool behavior has reached a steady-state configuration (Fig. 4.2 (a)). Whereas, the
value of \( \bar{\gamma} = 1.03 \) corresponds to a location near the right free edge, where the temperatures at all depths within the melt pool increase slightly without any noticeable change in the melt pool size as the laser begins to approach the right free edge. This value of \( \bar{\gamma} = 1.03 \) represents the last x-location where the nodes through the depth of the melt pool solidify before the laser is turned off. The melt pool at this location is therefore referred to as a transient melt pool. Finally, the values of \( \bar{\gamma} = 0.34 \) and \( \bar{\gamma} = 0 \) correspond to locations near and at the free edge of the wall which solidify as part of the stationary melt pool after the laser is turned off. The melt pool at these locations is referred to as a stationary melt pool.

Results for solidification cooling rates and thermal gradients extracted from the Rosenthal process maps of Figs. 2.3 and 2.4 (same \( T_m \) and the same normalized nodal locations as in the FEM model) are also plotted as a function of relative depth within the melt pool in Figs. 4.4 and 4.5, respectively. The Rosenthal solution is no longer valid upon approaching the free edge, as semi-infinite conditions cease to exist at these locations. Therefore, FEM results are only extracted from the locations \( \bar{\gamma} = 1.03 \) (approaching the free edge), \( \bar{\gamma} = 0.34 \) and \( \bar{\gamma} = 0 \) (near and at the free edge respectively).

![Figure 4.4: Effect of Melt Pool Behavior on Normalized Cooling Rate](image-url)
The results of Figs. 4.4 and 4.5 indicate that for a melt pool that has reached a steady-state configuration ($\lambda = 17.22$), the values of solidification cooling rates and thermal gradients extracted from finite element models with temperature-independent properties are within 1-2% of the values obtained using the analytical Rosenthal solution, at the same normalized depths within the melt pool.

The dimensionless cooling rate plot (Fig. 4.4) reveals that the cooling rate values for a transient melt pool ($\lambda = 1.03$) are lower than the cooling rate values for a steady-state melt pool ($\lambda = 17.22$). This is reasoned as follows: for a transient melt pool there is a slight increase in temperatures at all depths within the melt pool (when compared to the steady-state melt pool) without any noticeable change in melt pool size. An increase in temperature is analogous to an increase in power under steady state conditions, which would result in a decrease in cooling rates. However, the cooling rate values for a stationary melt pool ($\lambda = 0.34$ and $\lambda = 0$) fall in between those of a transient melt pool ($\lambda = 1.03$) and a steady-state melt pool ($\lambda = 17.22$). This is because even though there is an significant increase in melt pool size upon approaching the free edge, the laser is turned off at $\lambda_f = 0$. Shutting of the laser upon reaching the free edge is analogous to both decreasing the laser power (from a certain value to zero) and decreasing the laser velocity (again from a certain value.
to zero). Under steady-state conditions, decreasing laser power results in an increase in cooling rates, while decreasing laser velocity results in a decrease in cooling rates, which is a competing effect. However, the slight increase in cooling rates for a stationary melt pool when compared to the transient melt pool suggests a predominant effect of the equivalent decrease in laser power.

In contrast, the dimensionless thermal gradient plot of Fig. 4.5 reveals a very minor difference in the magnitudes of thermal gradients between the transient and steady-state melt pools. Again, in contrast to the behavior of the dimensionless cooling rates, the dimensionless thermal gradient values for a stationary melt pool are lower when compared to the thermal gradient values from both the steady-state and transient melt pools. This is because of the significant increase in melt pool size upon reaching the free edge, which is analogous to increasing the laser power under steady-state conditions. As discussed in chapter 2, increasing laser power (or decreasing $T_m$) results in a substantial decrease in thermal gradients at all depths within the melt pool.

### 4.1.4 Effect of Melt Pool Behavior on Grain Morphology in Ti-6Al-4V

This section presents the effect of melt pool behavior (steady-state vs. transient vs. stationary) on grain morphology in the Ti-6Al-4V material system. An important point to reiterate here is that the results are extracted from finite element simulations which include the nonlinear effects of temperature-dependent properties and latent heat of transformation of Ti-6Al-4V. As presented in chapters 2 and 3 of this dissertation, results for solidification thermal gradient and cooling rate can be interpreted in the context of a solidification map to provide predictions of grain morphology in laser-deposited Ti-6Al-4V. Upon extracting the solidification cooling rate $\frac{dT}{dt}$ and thermal gradient $|\nabla T|$ from the finite element simulations with temperature-dependent properties and latent heat effects, the solidification velocity $R$ is determined using equation 2.20. Next, by plotting the points on the $G$ vs. $R$ space, the expected grain morphology can be predicted as either equiaxed, columnar or mixed.

#### 4.1.4.1 Solidification Map Predictions

Solidification map showing the effect of melt pool behavior on grain morphology is shown in Fig. 4.6. Here again, the results are extracted at the same x-locations in the model represented by $\frac{a}{l}$.
The absorbed laser power ($\alpha Q = 122.5 \text{ W}$) and velocity ($V = 8.47 \text{ mm/s}$) considered here are the same as those used previously in the temperature-independent simulations, and are typical of those used in LENS$^\text{TM}$ deposition of thin-wall geometries [17].

![Graph showing grain morphology vs. melt pool behavior](image)

Figure 4.6: Effect of Melt Pool Behavior on Grain Morphology in Ti-6Al-4V
($Q = 350 \text{ W}, V = 8.47 \text{ mm/s}$)

From Fig. 4.6, it is clear that the data points from the steady-state melt pool behavior fall in the fully columnar region. This result is in agreement with that presented in chapters 2 and 3 of this dissertation. Next, the data points from the transient melt pool behavior also fall in the fully columnar region. This can be reasoned as follows: for the transient melt pool behavior there is a decrease in cooling rates without any noticeable change in thermal gradients (when compared to the steady-state melt pool). This results in a very small leftward movement in $G$ vs. $R$ space, and therefore all the data points from the transient melt pool also fall in the fully columnar region.
However, for the case of a stationary melt pool, there is a clear movement of the data points into the fully equiaxed region. This trend can be reasoned as follows: the significant increase in melt pool size upon reaching the free edge is analogous to increasing laser power under steady-state conditions. As previously discussed, an increase in laser power acts to reduce the thermal gradients at all depths within the melt pool, which for a fixed cooling rate would move the data down and to the right in the $G$ vs $R$ space. At the same time, the solidification rate $R$ decreases with an increase in laser power, which is a competing effect. However, the decrease in thermal gradients is more pronounced (by an order of magnitude) and dominates the effect.

### 4.1.5 Return From the Right Edge

This section presents the results for the laser reaching the right free edge, then traveling back toward the left free edge. Here, the effects of steady-state and transient melt pool behavior on solidification cooling rates and thermal gradients will be investigated. Figure 4.7 illustrates the return of the laser back from the right free edge. An important point to note in Fig. 4.7 is that the melt pool region is zoomed for a better view. Again as in Figure 3.2, the location of the laser in Fig. 4.7 is evident from the intensity of the temperature distribution. As the laser moving with a constant power and velocity approaches the right free edge of the wall (Fig. 4.7 (a)), there is an increase in melt pool size when compared to the melt pool size under steady-state conditions. Now, as the laser begins to travel back towards the left, the melt pool size becomes larger and larger when compared to that approaching the free edge (Fig. 4.7 (a) vs. 4.7 (b), (c), (d) and (e)). This is due to the preheating achieved when the laser initially approaches the free edge.

Here, the transient melt pool behavior as the laser begins its travel back from the right free edge will be studied. Solidification cooling rates and thermal gradients are extracted from this transient melt pool and are compared with their values from the steady-state melt pool. As in the previous section, the extracted values of solidification cooling rates and thermal gradients are normalized using the nondimensionalization scheme based on the analytical Rosenthal solution that was presented earlier (equation 2.8).
4.1.5.1 Results for Case II

Values of dimensionless cooling rates and thermal gradients are plotted as a function of relative depth within the melt pool (Figs. 4.8 and 4.9) at four different x-locations in the model as represented by $\frac{\bar{a}}{\bar{l}}$. Here again, $\bar{a}$ is the normalized distance from the right free edge and $\bar{l}$ is the steady-state melt pool length determined using the Rosenthal solution. As in the previous section, the value of $\frac{\bar{a}}{\bar{l}} = 17.22$ corresponds to a location at the center of the wall where the melt pool behavior has reached a steady-state configuration (during the initial travel of the laser from the left free
edge towards the right free edge). Whereas, the value of $\frac{\tau}{T} = 1.03$ corresponds to a location near the right free edge (during the initial travel of the laser towards the right free edge), where there is a slight increase in temperatures at all depths within the melt pool, without any noticeable change in the size of the melt pool. This value of $\frac{\tau}{T} = 1.03$ represents the last x-location where the nodes throughout the depth of the melt pool solidify before the laser begins its travel back from the right free edge. The melt pool at this location is considered a transient melt pool. At the x-locations $\frac{\tau}{T} = 17.22$ and $\frac{\tau}{T} = 1.03$, the solidification cooling rates and thermal gradients are the same as those presented in Figs. 4.4 and 4.5. This data is presented again for ease of comparison with the transient melt pool behavior during the travel of the laser back from the right free edge. The values of $\frac{\tau}{T} = 0.34$ and $\frac{\tau}{T} = 0$ correspond to locations near and at the right free edge of the wall, which solidify as a transient melt pool after the laser passes through these locations during its travel back from the right free edge.

![Figure 4.8: Effect of Melt Pool Behavior on Normalized Cooling Rate](image)

Figure 4.8: Effect of Melt Pool Behavior on Normalized Cooling Rate
The results of Figs. 4.8 and 4.9 indicate that the values of solidification cooling rates and thermal gradients of the transient melt pool behavior during the laser return ($\frac{\alpha}{\mathcal{T}} = 0.34$ and $\frac{\alpha}{\mathcal{T}} = 0$) are much lower than the values of steady-state melt pool behavior ($\frac{\alpha}{\mathcal{T}} = 17.22$) or the transient melt pool behavior during the initial approach towards the right free edge ($\frac{\alpha}{\mathcal{T}} = 1.03$). As shown in Fig. 4.7 there is a very significant increase in melt pool size during the return of the laser back from the right free edge. Coupled with the initial preheating during the lasers approach, this acts to reduce both cooling rates and thermal gradients.

4.2 Effects Near the Free Edge in Bulky 3-D Geometries

4.2.1 Modeling Approach

In this section, the bulky 3-D geometry of Fig. 2.2 is considered. The modeling assumptions are analogous to those presented in section 3.4 and hence will not be discussed here. However, in order to reduce computational time, a 2-D axisymmetric Finite Element (FE) model is used instead of a 3-D FE model. Such 2-D axisymmetric FE models have been used in the literature in place of 3-D
FE models for understanding both the process scaling [101] and transient effects [102] in the study of laser additive manufacturing processes. The 2-D axisymmetric models used here are similar to the ones used by Birnbaum et. al., [101] and Aggarangsi et. al., [102]. Since the 3-D Rosenthal solution is axisymmetric, there is no error introduced by the 2-D axisymmetric modeling.

A representative finite element mesh and boundary conditions for a 2-D axisymmetric model is shown in Fig. 4.10. The axisymmetric condition is applied on the z-axis (Fig. 4.10) which is parallel to the direction of laser travel. As stated in [101, 102], the 2-D axisymmetric model simulates the movement of the point heat source through the center of a large solid (twice the geometry of the actual volume is modeled) and hence the applied power here should be two times the power applied in a regular 3-D model. The models used here take this into account by using an $\alpha = 0.70$ instead of $\alpha = 0.35$ as used previously in the 3-D model. Steady-state results for solidification cooling rates and thermal gradients from the 2-D axisymmetric FE model were compared with the results from the 3-D FE model of chapter 3, which demonstrated less than 1% difference between the two methods.

Again as in the thin-wall model, the 2-D axisymmetric model has three different mesh densities going from left to right (in the x-direction). A coarser mesh is used for the first sixth of the model, while the element size in the next sixth of the model is one half of that in the coarser region. Finally, the remaining portion of the model has a finer mesh, where the element size is one fourth that of the coarser region. A fine (higher) mesh density is only used in the regions where solidification cooling rate and thermal gradient results are extracted. Further, as results from transient conditions are intended to be compared with results from steady-state conditions, a higher mesh density is also used at the center of the wall. Finally, the mesh uses a 4 noded linear axisymmetric heat transfer quadrilateral element, and has been modeled using the software package ABAQUS.

Figure 4.10: Representative 2-D Axisymmetric Thermal Finite Element Mesh [100–102]
In this section, thermal finite element analysis is carried out to model the movement of the laser beginning at the left free edge of the wall, traveling left to right across the wall and reaching the right free edge. Once the laser reaches the right free edge it is turned off. Here again, the effects of steady-state, transient and stationary melt pool behavior on solidification cooling rates and thermal gradients are investigated. Simulation results are presented for both temperature-independent and temperature-dependent (Ti-6Al-4V) properties. Results from simulations with temperature-independent properties are presented in nondimensional form, while the results from simulations with temperature-dependent properties are plotted on the solidification map for Ti-6Al-4V.

Here again as in sections 2.1 and 3.1, it is assumed that the dimensions of the model are sufficiently large such that the 3-D Rosenthal solution is applicable under steady-state conditions.

### 4.2.2 Nondimensionalization Scheme

This section describes the nondimensionalization scheme used for presenting the results from temperature-independent simulations. The nondimensionalization scheme is based on the 3-D analytical Rosenthal solution for a point heat source traversing a semi-infinite solid. Since the Rosenthal solution was discussed in detail in chapter 2 of this dissertation, it will only be described here as required.

Based on the 3-D Rosenthal solution, the normalized melting temperature is defined in equation 2.19 and is repeated here for convenience:

\[ T_m = \frac{T_m - T_0}{\left(\frac{\alpha Q}{\pi k}\right)\left(\frac{\rho c V}{2k}\right)} \]  

(4.2)

Finite element simulations with temperature-independent properties are run for a representative case of the process variables: absorbed laser power \( \alpha Q = 192.5 \) (\( \alpha = 0.35, Q = 550 \text{ W} \)) and laser velocity \( V = 8.47 \text{ mm/s} \) which corresponds to a \( T_m = 0.23 \). Solidification cooling rates and thermal gradients are then extracted from the 2-D axisymmetric model at various nodal locations through the depth of the melt pool using equations 3.1 and 3.2, respectively. Upon extraction, the solidification cooling rates and thermal gradients are nondimensionalized using equation 2.18. The dimensionless cooling rates and thermal gradients are then plotted as a function of relative depth within the melt pool, \( \frac{z_0}{z_m} \). The non-dimensional variable \( z_0 \) is the normalized nodal distance and \( z_m \) is the deepest extent of the melt pool for the given value of \( T_m = 0.23 \).
4.2.3 Results

Values of dimensionless cooling rates and thermal gradients are plotted as a function of relative depth within the melt pool in Figs. 4.11 and 4.12 at four different x-locations in the model as represented by $\bar{a}$. Here again, $\bar{a}$ is the normalized distance from the right free edge and $\bar{l}$ is the steady-state melt pool length as determined using the 3-D Rosenthal solution. The value of $\bar{a} = 10.76$ corresponds to a location at the center of the wall, where the melt pool behavior has reached a steady-state configuration. The value of $\bar{a} = 0.75$ corresponds to a location near the right free edge, where there is a slight increase in temperatures at all depths within the melt pool without any noticeable change in the shape of the melt pool. This value of $\bar{a} = 0.75$ represents the last x-location where the nodes through the depth of the melt pool solidify before the laser reaches the edge. The melt pool at this location is therefore referred to as transient melt pool. Finally, the values of $\bar{a} = 0.22$ and $\bar{a} = 0$ correspond to locations near and at the free edge which solidify as a stationary melt pool once the laser is turned off. The melt pool at these locations is referred to as a stationary melt pool.

Results for solidification cooling rates and thermal gradients extracted from the Rosenthal process maps of Figs. 2.5 and 2.6 (same $T_m$ and the same normalized nodal locations as in the FEM model) are also plotted for comparison.
The results of Figs. 4.11 and 4.12 indicate that for a melt pool that has reached a steady-state...
configuration, the values of solidification cooling rates and thermal gradients extracted from the finite element models with temperature-independent properties are within 1-2% of the values obtained using the analytical 3-D Rosenthal solution. The results of Figs. 4.11 and 4.12 reveal that for a transient melt pool \((\frac{\tau}{\eta} = 0.75)\), trends in dimensionless cooling rates and thermal gradients are similar to those observed for thin-wall geometries in Figs. 4.4 and 4.5. However, the dimensionless cooling rate values for a stationary melt pool \((\frac{\tau}{\eta} = 0.22 \text{ and } \frac{\tau}{\eta} = 0)\) are higher than the values from both transient \((\frac{\tau}{\eta} = 1.03)\) and steady-state \((\frac{\tau}{\eta} = 10.76)\) melt pools, while the dimensionless thermal gradient follows the same trend as in 2-D thin-wall geometries. This behavior of the dimensionless cooling rates is due to the availability of more directions for heat transfer in 3-D geometries, as compared to 2-D thin-wall geometries.

4.2.4 Effect of Melt Pool Behavior on Grain Morphology in Ti-6Al-4V

A solidification map showing the effect of melt pool behavior on grain morphology is shown in Fig. 4.13. The results are extracted at the same x-locations in the model as represented by \(\frac{\tau}{\eta}\). The fraction of the absorbed laser power \((\alpha Q = 192.5 \text{ W})\) and velocity \((V = 8.47 \text{ mm/s})\) considered here are the same as those used in the temperature-independent simulations presented in the previous section.
From Fig. 4.13 it is clear that the data points from the steady-state melt pool behavior fall in the fully columnar region. This result is in agreement with that presented in chapters 2 and 3 of this dissertation. Next, the data points from the transient melt pool behavior also fall in the fully columnar region. This trend is in keeping with the $G$ vs. $R$ predictions reported earlier in this chapter for thin-wall geometries. Finally, there is a clear movement of the data points from the stationary melt pool towards the boundary of fully columnar/mixed morphology and mixed/fully equiaxed morphology and further into the fully equiaxed region. Again this trend is also in keeping with the $G$ vs. $R$ predictions reported earlier for thin-wall geometries. Hence, results suggest a transition to mixed or fully equiaxed microstructure near the free edge.
4.3 Chapter Summary

In this chapter, the effect of melt pool behavior in the vicinity of a free edge on solidification cooling rates and thermal gradients has been investigated in both 2-D thin-wall and bulky 3-D geometries through thermal finite element analysis. Dimensionless cooling rates and thermal gradients extracted from finite element simulations with temperature-independent properties were plotted as a function of relative depth within the melt pool. Solidification cooling rates and thermal gradients extracted from simulations with temperature-dependent material properties for Ti-6Al-4V were then interpreted in the context of a solidification map for predicting trends in grain morphology in laser-deposited Ti-6Al-4V. Results suggest a transition from columnar to mixed or fully equiaxed microstructure at the free edge.
5 Effect of Laser Beam Width and Shape on Melt Pool Geometry and Microstructure

Thermal process maps for solidification cooling rate and thermal gradient based on the Rosenthal 2-D and 3-D point source solutions have been presented in chapter 2 of this dissertation. Results from these thermal process maps, when interpreted in the context of a solidification map for the Ti-6Al-4V material system, have clearly validated the utility of the Rosenthal solution for predicting trends in solidification microstructure in laser-deposited materials. However, in reality the laser beam is not a point source. Rather, it has either a circular or a square beam profile with a finite width. Also, with the advent of electron beam manufacturing or other next-generation processes, users may have more control over the distribution of incident energy, compared to laser based manufacturing. As a result, the ability to change the distribution of power (e.g., through changes in beam width) represents an additional process variable.

Among the key deposit characteristics, the control of melt pool size assumes the highest priority within the manufacturing community. This is because a consistent melt pool size is needed before specific features can even be built. At the same time, the control of microstructure is also critical, particularly in aerospace and other structural applications that have strict guidelines on resulting mechanical properties. While the control of melt pool size and solidification microstructure have been addressed in the literature [114], their interconnection has yet to be fully investigated. In particular, it has not been shown how changing process variables to control melt pool size might simultaneously affect cooling rates and thermal gradients which ultimately control microstructure.

To this end, this chapter presents the effects of a distributed heat source on melt pool geometry (length and depth) and the thermal conditions controlling microstructure (cooling rates and thermal gradients) in beam-based solid freeform fabrication. The approach is based on superposition of the
well known Rosenthal solution for a moving point heat source traversing an infinite substrate [60].

5.1 Superposition of Rosenthal 2-D Solution: Formulation for 2-D Thin Wall Geometry

This section presents the formulation for a uniform power distribution of finite width \( w \) by superposition of the Rosenthal 2-D point source solution for 2-D thin-wall geometries.

As previously noted, the Rosenthal 2-D point source solution in dimensionless form is given by

\[
\mathcal{T} = e^{-x_0} K_0(\sqrt{x_0^2 + z_0^2}).
\] (5.1)

When the beam is modeled as a distributed heat source, the absorbed power \( \alpha Q \) is distributed over a width \( \bar{w} \) as shown in Figure 5.1. The resulting distributed heat source is \( q = \alpha Q / \bar{w} \). Analogous to the spacial normalization presented in chapter 2 of this dissertation, the normalized beam width \( \bar{w} \) is defined as

\[
\bar{w} = \frac{w}{2k \rho c V}.
\] (5.2)

![Figure 5.1: Illustration of the Absorbed Laser Power \( \alpha Q \) Distributed Over a Width \( \bar{w} \)]

Now at a distance \( \bar{s} \) from the \( \bar{z}_0 \) axis, the distributed load \( q(\bar{s}) \, d\bar{s} \) acts as a point heat source, as shown in figure 5.2.
In Figure 5.2, the magnitude of the cross hatched region \( q(\vec{s}) \, d\vec{s} \) represents the magnitude of a single point heat source. The solution corresponding to each point heat source given by \( q(\vec{s}) \, d\vec{s} \) can be obtained by replacing \( \vec{x}_0 \) with \( (\vec{x}_0 - \vec{s}) \) in the dimensionless 2-D Rosenthal solution, i.e.,

\[
T = \frac{\pi kb}{q(\vec{s})} (T - T_0) = e^{-\left[(\vec{x}_0 - \vec{s})\right]} K_0 \left( \sqrt{(\vec{x}_0 - \vec{s})^2 + z_0^2} \right).
\]  

(5.3)

Letting \( q(\vec{s}) = \frac{\alpha Q}{w} \) in equation (5.3) gives

\[
T = \frac{\pi kb}{\frac{\alpha Q}{w}} (T - T_0) = e^{-\left[(\vec{x}_0 - \vec{s})\right]} K_0 \left( \sqrt{(\vec{x}_0 - \vec{s})^2 + z_0^2} \right).
\]  

(5.4)

The total solution can be obtained by superposing all the point heat sources \( q(\vec{s}) \, d\vec{s} \) between \(-\frac{w}{2}\) and \(\frac{w}{2}\), i.e.,

\[
T = \frac{\pi kb}{\alpha Q} (T - T_0) = \frac{1}{w} \int_{-\frac{w}{2}}^{\frac{w}{2}} e^{-\left[(\vec{x}_0 - \vec{s})\right]} K_0 \left( \sqrt{(\vec{x}_0 - \vec{s})^2 + z_0^2} \right) d\vec{s},
\]  

(5.5)

or

\[
T = \frac{1}{w} \int_{-\frac{w}{2}}^{\frac{w}{2}} e^{-\left[(\vec{x}_0 - \vec{s})\right]} K_0 \left( \sqrt{(\vec{x}_0 - \vec{s})^2 + z_0^2} \right) d\vec{s}.
\]  

(5.6)

Now for the purposes of numerical integration let
\[ \bar{s} = \frac{\overline{w}}{2} u, \quad (5.7) \]

or

\[ d\bar{s} = \frac{\overline{w}}{2} du. \quad (5.8) \]

Therefore when

\[ u = 1; \bar{s} = \frac{\overline{w}}{2} \quad \text{and} \quad u = -1; \bar{s} = -\frac{\overline{w}}{2}. \quad (5.9) \]

Hence equation (5.6) can now be written as

\[ \bar{T} = \frac{1}{\overline{w}} \int_{-1}^{1} e^{-(\overline{x}_0 - \frac{\overline{w}}{2} \xi)} K_0 \left( \sqrt{\frac{(\overline{x}_0 - \frac{\overline{w}}{2})^2 + \overline{z}_0^2}{2}} \right) \frac{1}{2} \overline{w} du, \quad (5.10) \]

or after canceling the \( \overline{w} \),

\[ \bar{T} = \frac{1}{2} \int_{-1}^{1} e^{-(\overline{x}_0 - \frac{\overline{w}}{2} \xi)} K_0 \left( \sqrt{\frac{(\overline{x}_0 - \frac{\overline{w}}{2})^2 + \overline{z}_0^2}{2}} \right) \frac{1}{2} \overline{w} du. \quad (5.11) \]

Equation (5.11) is the Rosenthal 2-D solution in dimensionless form for a uniform distributed heat source \( q = \frac{aQ}{\overline{w}} \).

The expressions for dimensionless cooling rate and thermal gradient are obtained by differentiating equation (5.11). The expression for dimensionless cooling rate is given by equation (5.12) and that for the dimensionless thermal gradient is given by equation (5.15) as follows:

\[
\frac{\partial \bar{T}}{\partial \overline{t}} = \frac{1}{2} \int_{-1}^{1} \left\{ e^{-(\overline{x}-\overline{t} - \frac{\overline{w}}{2})} K_1 \left( \sqrt{\frac{(\overline{x} - \overline{t} - \frac{\overline{w}}{2})^2 + \overline{z}_0^2}{2}} \right) \frac{\overline{x} - \overline{t} - \frac{\overline{w}}{2}}{\sqrt{\frac{(\overline{x} - \overline{t} - \frac{\overline{w}}{2})^2 + \overline{z}_0^2}}}ight.

\[ + e^{-\left(\overline{x} - \overline{t} - \frac{\overline{w}}{2}\right)} K_0 \left( \sqrt{\frac{(\overline{x} - \overline{t} - \frac{\overline{w}}{2})^2 + \overline{z}_0^2}{2}} \right) \} du, \quad (5.12)\]
\[
\frac{\partial T}{\partial x_0} = -\frac{1}{2} \int_{-1}^{1} \left\{ e^{-(x_0 - \frac{w}{2})} K_1 \left( \sqrt{\frac{(\sqrt{x_0 - \frac{w}{2}})^2 + z_0^2}{x_0 - \frac{w}{2}}} \right) - \frac{(x_0 - \frac{w}{2})}{\sqrt{(x_0 - \frac{w}{2})^2 + z_0^2}} \right\} \, du,
\]

\[
+ e^{-(x_0 - \frac{w}{2})} K_0 \left( \sqrt{\frac{(\sqrt{x_0 - \frac{w}{2}})^2 + z_0^2}{x_0 - \frac{w}{2}}} \right) \, du,
\]

(5.13)

\[
\frac{\partial T}{\partial z_0} = -\frac{1}{2} \int_{-1}^{1} \left\{ e^{-(x_0 - \frac{w}{2})} K_1 \left( \sqrt{\frac{(\sqrt{x_0 - \frac{w}{2}})^2 + z_0^2}{x_0 - \frac{w}{2}}} \right) - \frac{(z_0)}{\sqrt{(x_0 - \frac{w}{2})^2 + z_0^2}} \right\} \, du,
\]

(5.14)

and

\[
|\nabla T| = \sqrt{\left( \frac{\partial T}{\partial x_0} \right)^2 + \left( \frac{\partial T}{\partial z_0} \right)^2}.
\]

(5.15)

### 5.1.1 Results Illustrating the Effect of Beam Width

Results illustrating the effect of beam width are presented in this section. As in chapter 2 (results for point source), the results are presented in dimensionless form. Results illustrating the effect of normalized beam width on normalized melt pool length, normalized melt pool depth, normalized cooling rate and normalized thermal gradient are presented in Figs. 5.3, 5.4, 5.5 and 5.6. The normalized melt pool length and depth are plotted as a function of normalized beam width (Figs. 5.3 and 5.4) for different \( T_m \), whereas the normalized cooling rate and thermal gradient (Figs. 5.5 and 5.6) are plotted as a function of relative depth within the melt pool for different normalized beam widths for a specific value of \( T_m \). The definition of normalized melting temperature \( T_m \) is the same as used in chapter 2 for 2-D thin-wall geometries, and is provided below for reference purposes:

\[
T_m = \frac{T_m - T_0}{\alpha Q}.
\]

(5.16)

As outlined in chapter 2, changes in normalized melting temperature \( T_m \) correspond to changes in absorbed laser power (\( \alpha Q \)) for fixed material properties. In order to determine the melt pool geometry (length and depth), the coordinates \( (x_0, z_0) \) which lie on the boundary of the melt pool are
determined by replacing $T$ with the melting point $T_m$ and finding the roots of eq. (5.11) numerically. As in chapter 2, both the numerical integration and root finding are conducted using the software package MATLAB. The resulting normalized melt pool length $\bar{l}$ and normalized melt pool depth $\bar{d}$ are defined as

$$\bar{l} = \frac{l}{\frac{2k}{\rho c V}} \quad \text{and} \quad \bar{d} = \frac{d}{\frac{2k}{\rho c V}}. \quad (5.17)$$

The relative depth within the melt pool varies in the range $0 \leq \frac{z_0}{z_m} \leq 1$, where $z_0$ is a depth location in the melt pool and $z_m$ is the maximum depth of the melt pool for a given value of $T_m$ and $\overline{w}$.

---

**Figure 5.3:** Effect of Normalized Beam Width on Normalized Melt Pool Length for Different $T_m$

The results of Fig. 5.3, indicate that for a given value of $T_m$ (given laser power), the normalized melt pool length initially increases as the laser power is changed from a point source ($\overline{w} = 0$) to a uniformly distributed source of width $\overline{w}$. This is because spreading out the heat source initially heats more material along the length to temperatures above $T_m$. Also the shape of the melt pool is changed when the power distribution is changed from a point source to a uniform distributed source with a finite width. The melt pool is stretched out with more material being melted along the length.
when compared to the depth.

This increase in melt pool length continues until it reaches a maximum value at a specific value of $\overline{w}$. At this point, the heat flux becomes insufficient to melt any additional material along the length, so that subsequent increases in $\overline{w}$ result in a decrease in melt pool length. This decrease in melt pool length continues until the heat flux is no longer sufficient to melt any material at all, so that the melt pool ceases to exist ($\overline{d} \to 0$). Also, the curves corresponding to different $T_m$ in Fig. 5.3, indicate that the normalized width over which the same laser power can be distributed increases with decreasing $T_m$ (or increasing $\alpha Q$), and that the normalized melt pool length values increase with a decrease in $\overline{T}_m$ (or increase in $\alpha Q$).

Figure 5.4: Effect of Normalized Beam Width on Normalized Melt Pool Depth for Different $T_m$

In contrast to the normalized melt pool length, the normalized melt pool depth decreases monotonically with increasing $\overline{w}$ (Fig. 5.4). While spreading out the heat source initially melts more material in the length direction, the amount of heat available to melt the material through the depth decreases. As observed for melt pool length, this decrease in melt pool depth continues until the point when the melt pool ceases to exist ($\overline{d} \to 0$). Inspection of the ordinate scales in Figs.5.3 and 5.4 suggests that melt pool depth is more sensitive to changes in beam width compared to melt pool length; however, results also suggest that changing the beam width can have a significant effect on melt pool length, melt pool depth and the overall shape of the melt pool. Finally, the curves cor-
responding to different $\bar{T}_m$ in Fig. 5.4 also reveal an increase in normalized melt pool depth with decreasing $\bar{T}_m$ or increasing $\alpha Q$.

The effect of normalized beam width on normalized cooling rate and normalized thermal gradient for different $\bar{T}_m$ (different $\alpha Q$) is illustrated in Figs. 5.5 and 5.6. As discussed previously, here the normalized cooling rate and thermal gradient are plotted as a function of relative depth within the melt pool at different normalized beam widths for a given value of $\bar{T}_m$. The cooling rate and gradient curves corresponding to $\bar{w} = 0$ in Figs. 5.5 (a), (b), (c), (d) and 5.6 (a), (b), (c), (d) represent the cooling rates and gradients from the Rosenthal (point source) melt pool. An important point to note here is that for a given $\bar{T}_m$, the same relative depth location in the melt pool for different $\bar{w}$ does not correspond to the same location within the melt pool. This is because as discussed previously, when the laser power distribution is changed from a point source to a uniform distributed source with a finite width, there is a monotonic decrease in melt pool depth. The term $\bar{z}_m$ used in the relative depth definition represents the maximum depth of the melt pool for a given value of $\bar{w}$ and $\bar{T}_m$. Further, the cooling rate and gradient curves corresponding to different $\bar{w}$ plotted in Figs. 5.5 and 5.6, represent the values of $\bar{w}$ for which the left hand boundary (boundary where the solidification cooling rates and thermal gradients are extracted) of the melt pool at the surface is still outside the path of the beam. In accordance with the cooling rate and thermal gradient process map results of chapter 2, the cooling rate curves corresponding to different $\bar{w}$ in Fig. 5.5, reveal a decrease in cooling rate values through the depth of the melt pool, while the thermal gradient curves corresponding to different $\bar{w}$ in Fig. 5.6 reveal an increase in thermal gradient values through the depth of the melt pool.
Figure 5.5: Effect of Normalized Beam Width on Normalized Cooling Rate for Different $T_m$
Figure 5.6: Effect of Normalized Beam Width on Normalized Thermal Gradient for Different $T_m$

From Figs. 5.5 and 5.6 it is clear that the trends in dimensionless cooling rate and thermal gradient for different $w$ are nearly analogous for different $T_m$. In general, increasing $w$ results in an increase in both cooling rate and thermal gradient up to a certain depth within the melt pool, after which cooling rates and thermal gradients begin to decrease (relative to those for $w = 0$). This effect can be explained as follows. For the case of a point source ($w = 0$), the left hand boundary of the melt pool (i.e., the solidification boundary) is always relatively far from the heat source. As the laser power is distributed (increasing $w$), the solidification front near the surface begins to see the edge of the distributed source, which leads to an increase in both cooling rate and thermal gradient. However, beyond a certain depth within the melt pool (i.e., further away from the edge of the distributed source), bulk heating of the melt pool due to the distributed source results in a decrease in both cooling rate and thermal gradient compared to their point source counterparts. Still, both the

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solidification cooling rate and thermal gradient appear to be less sensitive to changes in laser beam width compared to the melt pool geometry (length and depth).

Finally, the variance of the cooling rates through the depth of the melt pool increases with increase in beam width for the same laser power (same $T_m$). Spreading the same laser power over a wide region is analogous to decreasing power (or increasing $T_m$). The cooling rate process map of chapter 2 (Fig. 2.3) reveals an increase in the variance of cooling rate through the depth of the melt pool with increasing $T_m$.

5.1.2 Representative Case for the Ti-6Al-4V Material System (Small-Scale LENS™ Deposition of Thin-Wall Geometries)

Results illustrating the effect of beam width, presented in the previous section are applicable for any material system since the Rosenthal solution assumes temperature-independent properties. In this section, the effect of beam width is investigated in laser-deposited Ti-6Al-4V. Here, the thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ$C are used to define both the normalized melting temperature and the spatial normalizations. Further, the values of laser power ($Q = 350$ W) and velocity ($V = 4.23$ mm/s) considered here fall in the range of powers and velocities that are typical of those used in the LENS™ deposition of thin-wall geometries. As in earlier chapters, the absorption coefficient is assumed to be $\alpha = 0.35$ and the wall thickness is assumed constant at $b = 2.26$ mm. The above values correspond to a dimensionless melting temperature $\bar{T}_m = 2.88$. Here again, results illustrating the effect of beam width are presented in dimensionless form. In the next section, the solidification cooling rate and thermal gradient results presented here will be interpreted in the context of a solidification map, to investigate the effect of beam width on trends in grain morphology in laser-deposited Ti-6Al-4V. When interpreting the results in the context of the solidification map, the dimensionless cooling rates and thermal gradients are converted to their actual values (equation. 2.8) using the thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ$C.

Results illustrating the effect of normalized beam width on normalized melt pool length, normalized melt pool depth, normalized cooling rates and normalized thermal gradients are plotted in Figs. 5.7 (a), (b), (c) and (d). Here again as in the previous section, the normalized melt pool length
and depth are plotted as a function of normalized beam width for the given value of $T_m$, while the
dimensionless cooling rates and thermal gradients are plotted as a function of relative depth within
the melt pool for different normalized beam widths for the given value of $T_m$. For the given velocity
and material properties, the results of Figs. 5.7 (a) and (b) correspond to actual beam widths in the
range $0 < w < 1.51 \, \text{mm}$.

Figure 5.7: Effect of Normalized Beam Width on (a) Normalized Melt Pool Length (b) Normalized
Melt Pool Depth (c) Normalized Cooling Rate (d) Normalized Thermal Gradient for $T_m = 2.88$

The results of Figs. 5.7 (a), (b), (c) and (d) indicate that the trends in normalized melt pool length,
depth, cooling rates and thermal gradients are similar to that observed in the previous section.
That
• The normalized melt pool length initially increases as the laser power is changed from a point source \((\overline{w} = 0)\) to a uniformly distributed source of width \(\overline{w}\), until it reaches a maximum value at a specific value of \(\overline{w}\). After this point, any subsequent increases in \(\overline{w}\) result in a decrease in melt pool length until the point when the power is no longer sufficient to melt the material (melt pool ceases to exist, \(l \rightarrow 0\)).

• The normalized melt pool depth monotonically decreases with increase in normalized beam width. Also, the melt pool depth is more sensitive to changes in beam width compared to melt pool length.

• The normalized cooling rate and thermal gradient increase with increasing \(\overline{w}\) up to a certain depth within the melt pool, after which cooling rates and thermal gradients begin to decrease (relative to those for \(\overline{w} = 0\)).

• The solidification cooling rate and thermal gradient appear to be less sensitive to changes in laser beam width compared to melt pool geometry (length and depth).

5.1.2.1 Effect of Beam Width on Grain Morphology (Small-Scale (LENS\textsuperscript{TM}) Deposition of Thin-Wall Geometries)

A solidification map showing the effect of beam width on grain morphology for small-scale (LENS\textsuperscript{TM}) deposition of thin-wall geometries is shown in Fig. 5.8. As discussed previously, the value of laser power and velocity considered here fall in the range that are typical of those used in the LENS\textsuperscript{TM} deposition of thin-wall geometries. Further, the values of \(G\) (thermal gradient) and \(R\) (solidification velocity which is the ratio of cooling rate to thermal gradient) plotted in Fig. 5.8 are extracted from the dimensionless cooling rate and thermal gradient plots of Figs. 5.7 (c) and (d), with thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature \(T_m = 1654^\circ\text{C}\). Here again as in chapters 2, 3 and 4, the fraction of the absorbed laser power is taken as \(\alpha = 0.35\).
From Fig. 5.8, it is clear that the data points corresponding to all beam widths and depths fall in the fully columnar region. This result is in keeping with the solidification map predictions reported for a point heat source in chapter 2, Cellular Automaton Solidification Modeling results [17] and experimental observations for LENS™ deposited Ti-6Al-4V [17,59]. Most importantly, the results of Fig. 5.8 reveal that the grain morphology is insensitive to beam width.

Analyzing the results from Figs. 5.7 (a), (b), (c) (d) and 5.8 reveals the following observations:

- Among the various key parameters in the laser deposition process, the melt pool depth is the most sensitive to beam width.

- The melt pool length initially increases, reaches a maximum value and then decreases with increase in beam width.
• The effect of beam width on solidification cooling rates and thermal gradients is not significant enough to cause any major changes in the trends in grain morphology in laser-deposited Ti-6Al-4V.

5.2 Superposition of Rosenthal 3-D Solution: Circular Beam Formulation for Bulky 3-D Geometry

This section presents the formulation for a uniform distribution of power over a circular beam of finite width w by superposition of the 3-D Rosenthal solution for a moving point heat source.

As previously discussed, the dimensionless 3-D Rosenthal solution for a moving point heat source traversing the top of a bulky 3-D geometry is given by

$$T = e^{-\left(\frac{x_0^2 + y_0^2 + z_0^2}{x_0^2 + y_0^2 + z_0^2}\right)} \frac{1}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}.$$  \hspace{1cm} (5.18)

When the laser is modeled as a uniform distributed heat source with a circular beam profile, the laser power \(\alpha Q\) is distributed over a circle of diameter \(W\) (Figure 5.9).
The distributed source $q$ is related to the total power $\alpha Q$ as

$$q = \frac{\alpha Q}{\pi w^2}. \quad (5.19)$$

Now consider a point source at a location $(\vec{r}, \theta)$ from the origin (i.e., in the $xy$ plane) (Figure 5.9(b)). As illustrated in Fig. 5.9 (b), the magnitude of a single point heat source corresponding to the distributed source $q$ is:
\[ qd\bar{A} = qrdrd\theta. \] (5.20)

Given the definition of \( T \), the Rosenthal 3-D solution of equation (5.18) can be written as

\[
\left( \frac{2\pi k^2}{\rho cV \alpha Q} \right) [T - T_0] = \frac{e^{-\left( x_0 + \sqrt{x_0^2 + y_0^2 + z_0^2} \right)}}{2 \sqrt{x_0^2 + y_0^2 + z_0^2}}.
\] (5.21)

Substituting \( \alpha Q = qrdrd\theta \), \( x_0 = x_0 - r \cos \theta \) and \( y_0 = y_0 - r \sin \theta \) into equation (5.21), the temperature corresponding to each point source \( qrdrd\theta \) is now given by

\[
\left( \frac{2\pi k^2}{\rho cV qrdrd\theta} \right) [T - T_0] = \frac{e^{-\left( (x_0 - r \cos \theta) + \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2} \right)}}{2 \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2}}.
\] (5.22)

Subbing \( q = \frac{4\alpha Q}{\pi \rho} \) in equation (5.22) gives

\[
\left( \frac{2\pi k^2}{\rho cV \frac{4\alpha Q}{\pi \rho} r drd\theta} \right) [T - T_0] = \frac{e^{-\left( (x_0 - r \cos \theta) + \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2} \right)}}{2 \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2}}.
\] (5.23)

The total solution due to the distributed source is obtained by summing all the point heat sources across the circular beam area.

i.e.,

\[
\frac{\pi \bar{w}^2}{4} \left( \frac{2\pi k^2}{\rho cV \alpha Q} \right) [T - T_0] = \int_0^{2\pi} \int_0^\pi e^{-\left( (x_0 - r \cos \theta) + \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2} \right)} \frac{r dr d\theta}{2 \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2}},
\] (5.24)

or equivalently,

\[
\bar{T} = 4 \frac{\pi \bar{w}^2}{\pi \rho} \int_0^{2\pi} \int_0^\pi e^{-\left( (x_0 - r \cos \theta) + \sqrt{(x_0 - r \cos \theta)^2 + (y_0 - r \sin \theta)^2 + (z_0)^2} \right)} r dr d\theta.
\] (5.25)

Now for the purposes of numerical integration, let

\[
\theta = \pi(u + 1) \quad \text{and} \quad \bar{T} = (v + 1)\bar{w},
\] (5.26)
so that

\[ d\theta = \pi du \quad \text{and} \quad d\tau = \frac{w}{4} dv. \quad (5.27) \]

Therefore, when

\[ \theta = 0; \ u = -1 \quad \text{and} \quad \theta = 2\pi; \ u = 1. \quad (5.28) \]

also, when

\[ \tau = 0; \ v = -1 \quad \text{and} \quad \tau = \frac{w}{2}; \ v = 1. \quad (5.29) \]

Equation (5.25) can now be written as

\[ \mathcal{T} = \frac{4}{\pi w^2} \int_{-1}^{1} \int_{-1}^{1} f(x) \left( \frac{v + 1}{w} \right) \pi du \frac{w}{4} dv, \quad (5.30) \]

where

\[
\begin{align*}
f(x) &= e^{-\left(\frac{y_0 - \frac{(v + 1)}{4} \cos[\pi(u + 1)]}{\left(\frac{y_0 - \frac{(v + 1)}{4} \cos[\pi(u + 1)]}{2} + \left(\frac{y_0 - \frac{(v + 1)}{4} \sin[\pi(u + 1)]}{2} + (z_0)^2\right)^2\right)\right)}}, \quad (5.31)
\end{align*}
\]

and

\[
\begin{align*}
g(x) &= 2\sqrt{\left(\frac{x_0 - \frac{(v + 1)}{4} \cos[\pi(u + 1)]}{2} + \left(\frac{y_0 - \frac{(v + 1)}{4} \sin[\pi(u + 1)]}{2} + (z_0)^2\right)^2\right)^2}. \quad (5.32)
\end{align*}
\]

Upon simplification, this gives

\[ \mathcal{T} = \frac{(v + 1)}{8} \int_{-1}^{1} \int_{-1}^{1} f(x) du dv. \quad (5.33) \]

Equation (5.33) is the Rosenthal 3-D solution in dimensionless form for a uniform distributed heat source with a circular beam shape.

The expressions for dimensionless cooling rate and thermal gradient can be obtained through differentiation of equation (5.33). The expression for dimensionless cooling rate is given by equation
(5.34) and the expression for dimensionless thermal gradient is given by equation (6.45).

Differentiating with respect to time gives

\[
\frac{\partial \mathcal{T}}{\partial t} = \frac{(v+1)}{8} \int_{-1}^{1} \int_{-1}^{1} c(x) \left\{ 1 + \frac{e(x)}{d(x)} + \frac{e(x)}{h(x)} \right\} dudv,
\]

(5.34)

where \(c(x), d(x), e(x)\) and \(h(x)\) are defined as

\[
c(x) = e \left\{ \left( \mathcal{V} - \mathcal{Y} \right) - \frac{(v+1)4\pi}{4} \cos(\pi(u+1)) \right\} + \sqrt{ \left( \mathcal{V} - \mathcal{Y} - \frac{(v+1)4\pi}{4} \cos(\pi(u+1)) \right)^{2} + (\mathcal{Y}_{0} - \frac{(v+1)4\pi}{4} \sin(\pi(u+1)))^{2} + (\mathcal{Y}_{0})^{2} \},
\]

(5.35)

\[
d(x) = \sqrt{ \left( \mathcal{V} - \mathcal{Y} - \frac{(v+1)4\pi}{4} \cos(\pi(u+1)) \right)^{2} + \left( \mathcal{Y}_{0} - \frac{(v+1)4\pi}{4} \sin(\pi(u+1)) \right)^{2} + (\mathcal{Y}_{0})^{2} \},
\]

(5.36)

\[
e(x) = \left[ \mathcal{V} - \mathcal{Y} - \frac{(v+1)4\pi}{4} \cos(\pi(u+1)) \right],
\]

(5.37)

\[
h(x) = \left[ \left( \mathcal{V} - \mathcal{Y} - \frac{(v+1)4\pi}{4} \cos(\pi(u+1)) \right)^{2} + \left( \mathcal{Y}_{0} - \frac{(v+1)4\pi}{4} \sin(\pi(u+1)) \right)^{2} + (\mathcal{Y}_{0})^{2} \right].
\]

(5.38)

also, differentiating with respect to \(\mathcal{Y}_{0}\) gives

\[
\frac{\partial \mathcal{T}}{\partial \mathcal{Y}_{0}} = -\frac{(v+1)}{8} \int_{-1}^{1} \int_{-1}^{1} f(x) \left\{ 1 + \frac{k(x)}{g(x)} + \frac{k(x)}{l(x)} \right\} dudv,
\]

(5.39)

where \(f(x)\) and \(g(x)\) are as defined in equations (5.31) and (5.32) respectively. Also in equation (5.39),

\[
k(x) = \left[ \mathcal{Y}_{0} - \frac{(v+1)4\pi}{4} \cos(\pi(u+1)) \right].
\]

(5.40)
\[ l(x) = \left[ \bar{x}_0 - \frac{(v+1)w}{4} \cos[\pi(u+1)] \right]^2 + \left( \bar{y}_0 - \frac{(v+1)w}{4} \sin[\pi(u+1)] \right)^2 + (\bar{z}_0)^2 \]. \quad (5.41)

Differentiating with respect to \( \bar{y}_0 \) gives

\[ \frac{\partial T}{\partial \bar{y}_0} = -\frac{(v+1)}{8} \int_{-1}^{1} \int_{-1}^{1} m(x) \frac{f(x)}{l(x)} \left\{ 1 + \left[ \frac{1}{g(x)} \right] \right\} dudv, \quad (5.42) \]

where

\[ m(x) = \left[ \bar{y}_0 - \frac{(v+1)w}{4} \sin[\pi(u+1)] \right]. \quad (5.43) \]

Finally, differentiating with respect to \( \bar{z}_0 \) gives

\[ \frac{\partial T}{\partial \bar{z}_0} = -\frac{(v+1)}{8} \int_{-1}^{1} \int_{-1}^{1} \bar{z}_0 \frac{f(x)}{l(x)} \left\{ 1 + \left[ \frac{1}{g(x)} \right] \right\} dudv. \quad (5.44) \]

Finally, the magnitude of the dimensionless thermal gradient is:

\[ \left| \nabla T \right| = \sqrt{\left( \frac{\partial T}{\partial \bar{x}_0} \right)^2 + \left( \frac{\partial T}{\partial \bar{y}_0} \right)^2 + \left( \frac{\partial T}{\partial \bar{z}_0} \right)^2}. \quad (5.45) \]

### 5.2.1 Results Illustrating the Effect of Beam Width for a Circular Laser Beam with a Uniform Intensity Distribution

Results illustrating the effect of beam width for a circular laser beam with a uniform intensity distribution are presented in this section. Here again, the results are presented in dimensionless form.

Results illustrating the effect of normalized beam width on normalized melt pool length, normalized melt pool depth, normalized cooling rate and normalized thermal gradient are presented in Figs. 5.10, 5.11, 5.12 and 5.13. As with the uniform distributed source results for thin-wall geometries, here again the normalized melt pool length and depth are plotted as a function of normalized beam width (Figs. 5.10 and 5.11) for different \( \bar{T}_m \), while the normalized cooling rate and thermal gradient (Figs. 5.12 and 5.13) are plotted as a function of relative depth within the melt pool for different normalized beam widths and for a specific value of \( \bar{T}_m \). The definition of normalized melting tem-
temperature \( T_m \) is the same as used in chapter 2 for bulky 3-D geometries, and is provided below for convenience:

\[
T_m = \frac{T_m - T_0}{\left(\frac{\alpha Q}{\pi r^2}\right) \left(\frac{\rho V}{2x}\right)}. \tag{5.46}
\]

As previously noted, changes in normalized melting temperature \( T_m \) correspond to changes in absorbed laser power \((\alpha Q)\) or laser velocity \(V\) for fixed material properties. The definitions of normalized melt pool length and normalized melt pool depth are the same as defined in equation 5.17. The relative depth within the melt pool varies in the range \(0 \leq \frac{z}{z_m} \leq 1\), where \(z_0\) is a depth location in the melt pool for a given value of \(T_m\), and \(z_m\) is the maximum depth of the melt pool for a given value of \(T_m\) and \(W\).

The results of Figs. 5.10, 5.11, 5.12 and 5.13 clearly show that the trends in normalized melt pool length, depth, cooling rates and thermal gradients for a circular laser beam with a uniform intensity distribution are very similar to the trends observed earlier for a uniform distributed heat source in 2-D, and hence will not be further discussed here.
Figure 5.10: Effect of Normalized Beam Width on Normalized Melt Pool Length for Different $T_m$

Figure 5.11: Effect of Normalized Beam Width on Normalized Melt Pool Depth for Different $T_m$
Figure 5.12: Effect of Normalized Beam Width on Normalized Cooling Rate for Different $T_m$
Figure 5.13: Effect of Normalized Beam Width on Normalized Thermal Gradient for Different $T_m$

5.2.2 Representative Case for Ti-6Al-4V Material System (Small-Scale LENS™ Deposition of Bulky 3-D Geometries)

The results presented in the previous section are applicable for any material system, since the Rosenthal solution assumes temperature-independent properties. In this section, the effect of beam width for a circular laser beam with a uniform intensity distribution is investigated specifically for laser-deposited Ti-6Al-4V. As with the representative Ti-6Al-4V case presented earlier for small-scale LENS™ deposition of thin-wall geometries, here again the thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ C$ are used to define both the normalized melting temperature and the spatial normalizations. Further, the values of laser power ($Q = 550 W$) and velocity ($V = 8.47 mm/s$) considered here fall in the range of powers and velocities that
are typical of those used in LENS\textsuperscript{TM} deposition of bulky 3-D geometries. Along with Ti-6Al-4V properties at $T_m = 1654^\circ$C, these values of power and velocity correspond to a dimensionless melting temperature $\overline{T}_m = 1.7$. Here again, results illustrating the effect of beam width are presented in dimensionless form. In the next section, the solidification cooling rate and thermal gradient results presented here will be interpreted in the context of a solidification map, to investigate the effect of beam width on trends in grain morphology in laser-deposited Ti-6Al-4V.

Results for Ti-6Al-4V illustrating the effect of normalized beam width on normalized melt pool length, normalized melt pool depth, normalized cooling rates and normalized thermal gradients are plotted in Figs. 5.14 (a), (b), (c) and (d). For the given process variables and material properties, the results of Figs. 5.14 (a) and (b) correspond to actual beam widths in the range of $0 < w < 2.0 \text{ mm}$. From Figs. 5.14 (a), (b), (c) and (d) it is clear that the trends in normalized melt pool length, depth, cooling rates and thermal gradients are similar to those observed earlier for small-scale LENS\textsuperscript{TM} deposition of thin-wall geometries and hence will not be discussed further.
5.2.2.1 Effect of Beam Width on Grain Morphology (Small-Scale LENS™ Deposition of Bulky 3-D Geometries)

A solidification map showing the effect of beam width on grain morphology for small-scale (LENS™) deposition of bulky 3-D geometries is shown in Fig. 5.15. The values of $G$ (thermal gradient) and $R$ (solidification velocity) plotted in Fig. 5.15 are extracted from the dimensionless cooling rate and thermal gradient plots of Figs. 5.14 (c) and (d), with thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ$C.
Figure 5.15: Effect of Beam Width (Circular Beam) on Grain Morphology in Ti-6Al-4V (Small-Scale (LENS™) Deposition of Bulky 3-D Geometries, Q = 550 W, V = 8.47 mm/s)

From Fig. 5.15, it is clear that the data points corresponding to all beam widths and depths fall in the fully columnar region. This result is in keeping with the solidification map predictions reported earlier for a point heat source in chapter 2, Cellular Automaton Solidification Modeling results [107] and experimental observations for LENS™ deposited Ti-6Al-4V [53–55, 58]. Again, the results of Fig. 5.15 reveal that the trends in grain morphology in laser-deposited Ti-6Al-4V are insensitive to beam width.

5.2.3 Representative Case for Ti-6Al-4V Material System (Large-Scale Deposition of Bulky 3-D Geometries)

In this section, the effect of beam width is investigated in large scale (higher-power) deposition of bulky 3-D geometries for a circular laser beam with a uniform intensity distribution. Again, the
thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ$C are used to define both the normalized melting temperature and the spatial normalizations. The values of laser power and velocity considered are 15000 W and 8.47 mm/s respectively. Along with Ti-6Al-4V properties at $T_m = 1654^\circ$C, these values of power and velocity correspond to a dimensionless melting temperature $T'_m = 0.06$. As presented earlier in this chapter, results illustrating the effect of beam width are presented in dimensionless form.

Results illustrating the effect of normalized beam width on normalized melt pool length, normalized melt pool depth, normalized cooling rates and normalized thermal gradients are plotted in Figs. 5.16 (a), (b), (c) and (d). From Figs. 5.16 (a), (b), (c) and (d) it is clear that the trends in normalized melt pool length, depth, cooling rates and thermal gradients are similar to those observed for small-scale LENS\textsuperscript{TM} deposition of bulky 3-D geometries. However, the ordinate scales indicate a substantial difference in magnitude, with an increase in melt pool length and depth and a decrease in both cooling rate and thermal gradient.
Figure 5.16: Effect of Normalized Beam Width on (a) Normalized Melt Pool Length (b) Normalized Melt Pool Depth (c) Normalized Cooling Rate (d) Normalized Thermal Gradient for a Large Scale Process ($\overline{T_m} = 0.06$)
5.2.3.1 Effect of Beam Width on Grain Morphology (Large-Scale Deposition of Bulky 3-D Geometries)

A solidification map showing the effect of beam width on grain morphology for large-scale (higher-power) deposition of bulky 3-D geometries is shown in Fig. 5.17. The values of $G$ and $R$ plotted in Fig. 5.17 are extracted from the dimensionless cooling rate and thermal gradient plots of Figs. 5.16 (c) and (d), with thermophysical properties of Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654$°C.

![Solidification Map](image)

Figure 5.17: Effect of Beam Width (Circular Beam) on Grain Morphology in Ti-6Al-4V (Large-Scale Deposition of Bulky 3-D Geometries, $Q = 15000$ W, $V = 8.47$ mm/s)

From Fig. 5.17, it is clear that the data points corresponding to all beam widths and depths reveal a graded microstructure through the depth of the deposit, with a mixed or even fully equiaxed microstructure at the surface. This result is in keeping with the solidification map predictions reported...
in chapter 2 (for a point heat source) for large-scale processes, Cellular Automaton Solidification Modeling results [107] and experimental observations reported in the literature for a 14 kW large-scale process [58]. Again, the results of Fig. 5.17 reveal that the trends in grain morphology in laser-deposited Ti-6Al-4V are insensitive to beam width.

### 5.3 Superposition of Rosenthal 3-D Solution: Square Beam

**Formulation for Bulky 3-D Geometries**

This section presents the formulation for a uniform distribution of power over a square beam of finite width \( w \) by superposition of the 3-D Rosenthal solution for a moving point heat source. As previously noted, the dimensionless Rosenthal 3-D solution for a point heat source moving across the top of a bulky 3-D geometry is given by equation (5.18) and is repeated here for convenience:

\[
T = e^{-\left(\frac{x_0 + \sqrt{x_0^2 + y_0^2 + z_0^2}}{2\sqrt{x_0^2 + y_0^2 + z_0^2}}\right)}.
\]

When the laser is modeled as a square beam, the absorbed laser power \( \alpha Q \) is distributed over a square of side \( \bar{w} \) (Figure 5.18).
Figure 5.18: Illustration of a Square Laser Beam with a Uniform Distributed Heat Source

The distributed heat source is \( q = \frac{\alpha q}{w^2} \), where \( w^2 \) is the area of a square.
The magnitude of the cross-hatched region \( q(\bar{s}, \bar{m}) \ d\bar{s} \ d\bar{m} \) in Fig. 5.18 (b) is the magnitude of a single point heat source acting at a location \((\bar{s}, \bar{m})\). If the coordinate system is placed at the location of the point source \( q(\bar{s}, \bar{m}) \ d\bar{s} \ d\bar{m} \), then \( \bar{x}_0 = (\bar{x}_0 - \bar{s}) \) and \( \bar{y}_0 = (\bar{y}_0 - \bar{m}) \). The Rosenthal 3-D solution in dimensionless form can now be written as

\[
\left( \frac{2 \pi k^2}{\rho c V q d\bar{s} d\bar{m}} \right) \ [T - T_0] = e^{-\{ (\bar{x}_0 - \bar{s}) + \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0} \}} \\
\frac{2}{2 \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0}}. \tag{5.47}
\]

The point heat source \( q(\bar{s}, \bar{m}) \ d\bar{s} \ d\bar{m} \) can also be written as

\[
q(\bar{s}, \bar{m}) \ d\bar{s} \ d\bar{m} = \frac{\alpha Q}{\bar{w}^2} \ d\bar{s} \ d\bar{m}. \tag{5.48}
\]

Subbing equation (5.48) into equation (5.47) gives

\[
\left( \frac{2 \pi k^2}{\rho c V \frac{\alpha Q}{\bar{w}^2} \ d\bar{s} \ d\bar{m}} \right) \ [T - T_0] = e^{-\{ (\bar{x}_0 - \bar{s}) + \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0} \}} \\
\frac{2}{2 \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0}}. \tag{5.49}
\]

or

\[
\frac{\bar{w}^2}{d\bar{s} d\bar{m}} \left( \frac{2 \pi k^2}{\rho c V \frac{\alpha Q}{\bar{w}^2}} \right) \ [T - T_0] = e^{-\{ (\bar{x}_0 - \bar{s}) + \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0} \}} \\
\frac{2}{2 \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0}}. \tag{5.50}
\]

The total solution can then be obtained by superposing all point source solutions between \( \frac{-\bar{x}}{2} \) \( \to \frac{\bar{x}}{2} \) and \( \frac{-\bar{m}}{2} \) \( \to \frac{\bar{m}}{2} \), i.e.,

\[
[T] = \frac{1}{\bar{w}^2} \int_{-\frac{\bar{x}}{2}}^{\frac{\bar{x}}{2}} \int_{-\frac{\bar{m}}{2}}^{\frac{\bar{m}}{2}} e^{-\{ (\bar{x}_0 - \bar{s}) + \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0} \}} \\
\frac{2}{2 \sqrt{(\bar{x}_0 - \bar{s})^2 + (\bar{y}_0 - \bar{m})^2 + \bar{z}_0}} \ d\bar{s} \ d\bar{m}. \tag{5.51}
\]

For the purposes of numerical integration, let

\[
\bar{s} = \frac{u \bar{w}}{2} \text{ and } \bar{m} = \frac{v \bar{w}}{2}, \tag{5.52}
\]

which gives

\[
d\bar{s} = \frac{1}{2} \ du \bar{w} \text{ and } d\bar{m} = \frac{1}{2} \ dv \bar{w}. \tag{5.53}
\]

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Therefore, when

\[ u = 1; \overline{\sigma} = \frac{w}{2} \] and when \[ u = -1; \overline{\sigma} = -\frac{w}{2}. \]  

(5.54)

Similarly, when

\[ v = 1; \overline{m} = \frac{w}{2} \] and when \[ v = -1; \overline{m} = -\frac{w}{2}. \]  

(5.55)

Hence, equation 5.51 can now be written as

\[ \overline{T} = \frac{1}{w} \int_{-1}^{1} \int_{-1}^{1} e^{\frac{1}{2} \left\{ \left( \overline{x}_0 - u \overline{z} \right)^2 + \left( \overline{x}_0 - v \overline{z} \right)^2 + \overline{z}_0 \right\}} \frac{1}{2} du dv \overline{w} \frac{1}{2} dv \overline{w}. \]  

(5.56)

Upon simplification

\[ \overline{T} = \int_{-1}^{1} \int_{-1}^{1} e^{\frac{1}{8} \left\{ \left( \overline{x}_0 - u \overline{z} \right)^2 + \left( \overline{x}_0 - v \overline{z} \right)^2 + \overline{z}_0 \right\}} du dv. \]  

(5.57)

Equation (5.57) is the dimensionless Rosenthal 3-D solution for a square laser beam with a uniform intensity distribution.

The expressions for dimensionless cooling rate and dimensionless thermal gradient can be obtained through differentiation of equation (5.57). The expression for dimensionless cooling rate is given by

\[ \frac{\partial \overline{T}}{\partial \tau} = \frac{1}{8} \int_{-1}^{1} \int_{-1}^{1} \frac{a(x)}{b(x)} \left\{ 1 + \frac{c(x)}{b(x)} \right\} du dv, \]  

(5.58)

where

\[ a(x) = e^{\frac{1}{8} \left\{ \left( \overline{x}_0 - u \overline{z} \right)^2 + \left( \overline{x}_0 - v \overline{z} \right)^2 + \overline{z}_0 \right\}}, \]  

(5.59)

\[ b(x) = \sqrt{\left( \overline{x} - \overline{u} \overline{w} / 2 \right)^2 + \left( \overline{y} - \overline{v} \overline{w} / 2 \right)^2 + \overline{z}_0^2}, \]  

(5.60)

\[ c(x) = \left[ \overline{x} - \overline{u} \overline{w} / 2 \right], \]  

(5.61)
and
\[
d(x) = \left[ \left( \overline{x} - \overline{y} - u \frac{W}{2} \right)^2 + \left( \overline{y}_0 - \overline{z} \frac{W}{2} \right)^2 + \overline{z}_0^2 \right]. \tag{5.62}
\]

The expression for dimensionless thermal gradient is obtained by differentiating in space, i.e.,
\[
\frac{\partial \overline{T}}{\partial \overline{x}_0} = -\frac{1}{8} \int_{-1}^{1} \int_{-1}^{1} e(x) \left\{ 1 + \frac{g(x)}{f(x)} + \frac{g(x)}{h(x)} \right\} dudv, \tag{5.63}
\]

where
\[
e(x) = e^{-\left\{ (\overline{x}_0 - u \frac{W}{2}) + \sqrt{(\overline{x}_0 - u \frac{W}{2})^2 + (\overline{y}_0 - v \frac{W}{2})^2 + \overline{z}_0^2} \right\}}, \tag{5.64}
\]

\[
f(x) = \sqrt{\left( \overline{x}_0 - u \frac{W}{2} \right)^2 + \left( \overline{y}_0 - v \frac{W}{2} \right)^2 + \overline{z}_0^2}, \tag{5.65}
\]

\[g(x) = \left[ \overline{x}_0 - u \frac{W}{2} \right], \tag{5.66}\]

and
\[
h(x) = \left[ \left( \overline{x}_0 - u \frac{W}{2} \right)^2 + \left( \overline{y}_0 - v \frac{W}{2} \right)^2 + \overline{z}_0^2 \right]. \tag{5.67}
\]

Similarly,
\[
\frac{\partial \overline{T}}{\partial \overline{y}_0} = -\frac{1}{8} \int_{-1}^{1} \int_{-1}^{1} i(x) \frac{e(x)}{h(x)} \left\{ 1 + \frac{1}{f(x)} \right\} dudv, \tag{5.68}
\]

where
\[
i(x) = \left[ \overline{y}_0 - v \frac{W}{2} \right]. \tag{5.69}\]

Finally,
\[
\frac{\partial \overline{T}}{\partial \overline{z}_0} = -\frac{1}{8} \int_{-1}^{1} \int_{-1}^{1} \overline{z}_0 \frac{e(x)}{h(x)} \left\{ 1 + \frac{1}{f(x)} \right\} dudv. \tag{5.70}
\]
The resulting dimensionless thermal gradient is

\[ |\nabla T| = \sqrt{\left(\frac{\partial T}{\partial x_0}\right)^2 + \left(\frac{\partial T}{\partial y_0}\right)^2 + \left(\frac{\partial T}{\partial z_0}\right)^2}. \]  

(5.71)

### 5.3.1 Representative Results Illustrating the Effect of Beam Width for a Square Laser Beam with a Uniform Intensity Distribution

In this section, results illustrating the effect of beam width for a square laser beam with a uniform intensity distribution are presented. In Fig. 5.19, the effect of normalized beam width on normalized melt pool length, depth, cooling rates and thermal gradients are presented for a specific value of \( T_m = 0.5 \). In Fig. 5.19, the melt pool length and depth are plotted as a function of normalized beam width, whereas the cooling rates and thermal gradients are plotted as a function of relative depth within the melt pool. The normalized melting temperature definition follows equation (5.46).

The results of Fig. 5.19 reveal that the trends in normalized melt pool length, depth, cooling rates and thermal gradients for a square laser beam with a uniform intensity distribution are very similar to trends observed earlier for a circular laser beam.
5.3.1.1 Effect of Beam Width on Grain Morphology (Small-Scale (LENS™))

Deposition of Bulky 3-D Geometries)

A solidification map showing the effect of beam width on grain morphology for small-scale (LENS™) deposition of bulky 3-D geometries is shown in Fig. 5.20. The values of laser power and velocity considered here are $Q = 550 \text{ W}$ and $V = 8.47 \text{ mm/s}$ respectively.
From Fig. 5.20, it is clear that the data points corresponding to all beam widths and depths fall in the fully columnar region. This result is in keeping with the solidification map predictions reported for a point heat source in chapter 2, the $G$ vs. $R$ predictions reported earlier for a circular laser beam (small-scale), Cellular Automaton Solidification Modeling results [107] and experimental observations for LENS™ deposited Ti-6Al-4V [53–55, 58]. Again, the results of Fig. 5.20 reveal that the trends in grain morphology in laser-deposited Ti-6Al-4V are insensitive to beam width.

5.3.1.2 Effect of Beam Width on Grain Morphology (Large-Scale Deposition of Bulky 3-D Geometries)

A solidification map showing the effect of beam width on grain morphology for large-scale (higher-power) deposition of bulky 3-D geometries is shown in Fig. 5.21. The values of laser power and
velocity considered here are $Q = 15000 \, W$ and $V = 8.47 \, mm/s$ respectively.

![Graph showing the effect of beam width on grain morphology in Ti-6Al-4V](image)

**Figure 5.21:** Effect of Beam Width (Square Beam) on Grain Morphology in Ti-6Al-4V (Large-Scale Deposition of Bulky 3-D Geometries, $Q = 15000 \, W$, $V = 8.47 \, mm/s$)

From Fig. 5.21, it is clear that the data points corresponding to all beam widths and depths reveal a graded microstructure through the depth of the deposit, with a mixed or even fully equiaxed microstructure at the surface. This result is in keeping with the solidification map predictions reported in chapter 2 (for a point heat source) for large-scale processes, $G$ vs. $R$ predictions reported earlier for a circular laser beam with uniform intensity distribution (large-scale processes), Cellular Automaton Solidification Modeling results [107] and experimental observations reported in the literature for a 14 $kW$ large-scale process [58]. The results of Fig. 5.21 also reveal that the trends in grain morphology in large-scale deposition of Ti-6Al-4V are insensitive to beam width.
5.4 Chapter Summary

In this chapter, superposition of the Rosenthal solution has been used to investigate the effect of beam width and shape on melt pool length, melt pool depth, solidification cooling rates and thermal gradients in both 2-D thin-wall and bulky 3-D geometries. In each case, a uniform intensity distribution is considered. In 3-D, two different beam shapes are considered: a circular laser beam and a square laser beam. Solidification cooling rates and thermal gradients are also interpreted in the context of a solidification map to investigate the effect of beam width and shape on trends in grain morphology in laser-deposited Ti-6Al-4V, for both small-scale (LENS\textsuperscript{TM}) and large-scale (higher power) processes. Results suggest that changes in beam width could have a significant effect on the melt pool geometry without affecting microstructure.
6 Summary and Contributions

6.1 Summary

The primary obstacles to the wide-spread commercialization of laser-based solid freeform fabrication processes, as a viable manufacturing alternative for metallic components, include the control of melt pool size, residual stress and microstructure [16]. The control of melt pool size and residual stress has recently been considered in the literature [18, 48–51], while the control of microstructure has not yet been addressed. This dissertation addresses this critical issue of the control of microstructure in laser-based solid freeform fabrication by using a combination of both analytical and numerical modeling approaches. To date, most of the progress in relating laser deposition process variables (e.g., laser power and velocity) to the resulting microstructure (e.g., grain size and morphology) has been limited to experimentation coupled with intuition, and suitable microstructures have typically been obtained only by trial and error [52, 54, 57–59]. In addition, it is unclear whether knowledge based on small-scale laser deposition processes (e.g., LENS™) can be applied to large-scale (higher power) processes currently under development for commercial application.

This dissertation thoroughly investigated the effects of process variables and size-scale on solidification microstructure, with specific application to the Ti-6Al-4V material system.

In this dissertation, thermal process maps for solidification cooling rate and thermal gradient (the key parameters controlling microstructure) have been developed based on the well known Rosenthal solution for a moving point heat source traversing an infinite substrate [60]. The process maps have been used to provide general insights into the roles of process variables and size-scale on microstructure in laser-deposited materials. Further, the nonlinear effects of temperature-dependent properties and latent heat have been included through thermal finite element modeling. In this dissertation, the primary purpose of finite element modeling has been to assess the validity of the
Rosenthal results for predicting trends in solidification microstructure. This has been investigated for small-scale (LENS™) deposition of thin-walled geometries, and both small-scale (LENS™) and large-scale (higher power) deposition of bulky 3-D deposits. Numerical results obtained from both the Rosenthal and FEM solutions have been plotted on solidification maps for predicting grain morphology in Ti-6Al-4V, and the utility of the Rosenthal solution for predicting trends in solidification microstructure has been verified.

The use of thermal process maps for predicting trends in solidification microstructure is a major contribution of this dissertation. A key point to consider here is that since the Rosenthal solution assumes temperature-independent properties, the thermal process maps that have been developed based on Rosenthal solution can be applied to any material system. Thermal process maps have been developed for two basic geometries, 2-D thin-walled and bulky 3-D structures. The process map for cooling rate, (which is largely responsible for grain size) and the process map for thermal gradient (which in combination with cooling rate is responsible for grain morphology) have been developed for both the geometries. From the thermal process maps, it has been shown that:

- Trends in both solidification cooling rate and thermal gradient are the same for both thin-wall and bulky geometries.
- For fixed material properties and laser velocity, changes in laser power can change both the dimensionless cooling rate and thermal gradient by several orders of magnitude in both 2-D and 3-D geometries.
- There is a significant variation of the dimensionless cooling rate throughout the depth of the melt pool in both 2-D and 3-D geometries.
- The dimensionless thermal gradient is relatively insensitive to depth in 2-D, while it is slightly more sensitive in 3-D.
- In 2-D, the actual cooling rate scales with the square of the laser velocity, while in 3-D it scales with the cube of the laser velocity.
- In 2-D, the actual thermal gradient scales linearly with laser velocity, while in 3-D it scales with the square of the laser velocity.
In both 2-D and 3-D, increasing laser power results in a substantial decrease in thermal gradient at all depths within the melt pool, while the cooling rate is most significantly affected at the surface. Therefore, increasing laser power (i.e., increasing process size scale) acts to decrease the high thermal gradients typically associated with a columnar microstructure, with an increase in solidification rate (ratio of cooling rate to thermal gradient) towards the surface of the deposit. This suggests the potential for a grading of the microstructure throughout the depth of the deposit, with a transition from columnar to equiaxed microstructure at the surface.

Thermal finite element analysis, which includes the nonlinear material behavior neglected by the Rosenthal solution, have clearly validated the trends in solidification microstructure predicted by the Rosenthal solution. In this dissertation, both the Rosenthal and FEM results for solidification cooling rate and thermal gradient have been compared and interpreted in the context of a solidification map for Ti-6Al-4V [53, 55, 56, 58, 61, 62]. In conclusion, although the Rosenthal results neglect the nonlinear effects of temperature-dependent properties and latent heat, trends in $G$ vs. $R$ data are in reasonable agreement with the FEM results. Moreover, the grain morphology predicted by both Rosenthal and FEM results are in agreement with experimental observations both for thin-wall [17, 59] and bulky deposits [53, 54, 58].

Thermal finite element analysis has also been used to generate previously unreported results on the effect of melt pool behavior, on solidification cooling rates and thermal gradients in the vicinity of a free edge. Results from finite element simulations with temperature-dependent properties and latent heat effects for Ti-6Al-4V have also been interpreted in the context of a solidification map to investigate the effect of the free edge on trends in grain morphology in laser-deposited Ti-6Al-4V. In conclusion, the increase in melt pool size upon reaching the free edge results in a significant decrease in thermal gradients, which results in net downward movement in $G$ vs. $R$ space.

Finally, superposition of the Rosenthal point source solution has been used to investigate previously unreported results for the effect of beam width and shape on melt pool length, depth, cooling rates and thermal gradients. Further, the results have been interpreted in the context of the solidification map to understand the effect of beam width and shape on trends in grain morphology in laser-deposited Ti-6Al-4V. Results indicate that:
• Melt pool geometry (both length and depth) is sensitive to changes in beam width.

• The effect of beam width and shape on solidification cooling rates and thermal gradients is not significant enough to cause any major changes in the trends in grain morphology in laser-deposited Ti-6Al-4V.

• Hence, results suggest that changes in beam width can be used to control melt pool geometry, without affecting microstructure.

6.2 Contributions of the Research

In summary, the contributions of this research are:

• Development of previously unreported thermal process maps for dimensionless solidification cooling rates and thermal gradients for both 2-D thin-walled and 3-D bulky structures. Based on the Rosenthal point source solution, these process maps fully map out the effects of the key laser deposition process variables (laser power and velocity) and size-scale on solidification microstructure in laser-deposited materials.

• Demonstration of the utility of the Rosenthal solution for predicting trends in solidification microstructure for both small-scale and large-scale processes.

• Further underscoring the utility of the solidification map approach for predicting trends in grain morphology in laser-processed materials, particularly Ti-6Al-4V.

• Presentation of previously unreported results for the effect of melt pool behavior on solidification cooling rates and thermal gradients (and thereby on the resulting microstructure) in the vicinity of the free edge.

• Presentation of previously unreported formulations for a uniform distributed heat source in both 2-D and 3-D based on the superposition of the 2-D and 3-D Rosenthal solution point source solution.

• Presentation of previously unreported results for the effect of laser beam width and shape on melt pool length, melt pool depth, solidification cooling rates, thermal gradients and finally
on the resulting microstructure in the Ti-6Al-4V material system.
The primary motivation for this dissertation was to develop simulation based methods that will fully investigate the effects of deposition process variables (e.g., laser power and velocity) and size-scale on the resulting microstructure. When this work started, there was no method that would thoroughly investigate the effects of process variables and size-scale on the resulting microstructure. All the available data and guidelines, relating the process variables to microstructure was experimental coupled with intuition. Therefore, to overcome these limitations on microstructure control, this dissertation proposed a combination of analytical and numerical modeling approaches to study the effects of key deposition process variables and size-scale on solidification microstructure, and thereby provide guidelines to control the microstructure. Inspite of all the progress made in the current research, the the work can be further extended in a few directions. The following tasks have been identified as future research directions.

- The thermal process maps developed in this dissertation are applicable to any material system. Till date, these thermal process maps have been used to provide predictions of trends in solidification microstructure for the Ti-6Al-4V material system. This was done by plotting the Rosenthal results of Figs. 2.3, 2.4, 2.5 and 2.6 on the solidification map of Ti-6Al-4V, with thermophysical properties for Ti-6Al-4V assumed constant at the melting temperature $T_m = 1654^\circ C$. As part of future work, these thermal process maps can be used to provide insights into trends in solidification microstructure for any material system, provided solidification maps are available for that material system.

- In Chapter 4 of this dissertation, thermal finite element analysis is used to investigate the effect of transient changes in melt pool size in the vicinity of the free-edge on solidification cooling
rates and thermal gradients (and thereby on the resulting microstructure). This approach can be extended to investigate the transient changes in solidification cooling rates and gradients due to step changes in laser power and velocity that was not addressed in this research.

- Chapter 5 of this dissertation, investigated the effect of a uniform distributed heat source on melt pool geometry (length and depth) and the thermal conditions controlling microstructure (cooling rates and thermal gradients) in beam-based solid freeform fabrication by superposition of the Rosenthal point source solution. As part of future work, this approach can be extended to investigate the effect of a heat source with Gaussian intensity distribution on melt pool geometry and microstructure for both 2-D thin wall and bulky 3-D geometries again by superposition of the Rosenthal solution.
A Matlab Code Listings for 2-D Rosenthal Solution

Listing A.1: Matlab File for Finding Roots (Melt Pool Dimensions)

```matlab
clc
clear all
close all

% Value of Tmbar
Tmbar = input('Please input the value of Tmbar = ');% Initial guess for root finding
x0bar(1) = input('Please input the initial guess for root finding = ');

% Resolution
a = input('Please input the resolution through the depth of the melt pool = ');

% Normalized melt pool depth
ND = input('Please input the melt pool depth = ');

% Variance of Normalized melt pool length (0 < d < L)
d = linspace(0,ND,a);
D = d';

% Initializations
m = 1;
NCR = zeros(1,a);

while m <= a
    % Normalized melt pool depth
    z0bar(m) = D(m);
    x(m) = fzero(@(x) f(x0bar(m),Tmbar,z0bar(m)), []);
    NCR(m) = exp(-x(m)) * (besselk(0,sqrt(x(m)^2 + z0bar(m)^2)) + (x(m)*besselk(1,sqrt(x(m)^2 + z0bar(m)^2)))) / (sqrt(x(m)^2 + z0bar(m)^2));
    x0bar(m+1) = x(m);
    z0(m) = z0bar(m)/ND;
    m = m + 1;
    n = n + 1;
end
```

Listing A.2: Matlab File for Equation Call

```matlab
function value = f(x0bar,Tmbar,z0bar)
value = Tmbar - (exp(-x0bar)*besselk(0,sqrt(x0bar^2 + z0bar^2)));
```

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Listing A.3: Matlab File for Evaluating Dimensionless and Actual Solidification Cooling Rates and Thermal Gradients

```matlab
clc
clear all

% Definition of constants
rho = input('Please input the value of mass density = ');
c = input('Please input the value of specific heat = ');
k = input('Please input the value of thermal conductivity = ');
v = input('Please input the value of velocity = ');
Tm = input('Please input the value of melting temperature = ');
T0 = input('Please input the initial temperature = ');
b = input('Please input the value of wall thickness = ');
alpha = 0.35; % Fraction of the absorbed laser power
tmpLP = input('Please input the value of laser power = ');
tmpx0bar = input('Please input the initial guess for root finding = ');
tmpnd = input('Please input the melt pool depth value = ');

for i = 1:size(tmpLP)
    Tmbar = ((pi*b*(Tm - T0))/(alpha*tmpLP(i)));
    x0bar(i) = tmpx0bar(i);

% Resolution
a = input('Please input the resolution through the depth of the melt pool = ');
% Normalized melt pool depth
ND = tmpnd(i)*input('Please input the melt pool depth = ');
% Variance of Normalized melt pool length (0 < d < L)
d = linspace(0,ND,a);
D = d';

% Initializations
m = 1;

while n <= a
    z0bar(m) = D(m);
    x(m) = fzero (@f, x0bar(m), [] , Tmbar, z0bar(m));

% Non-dimensional Cooling Rate
NCR(m) = exp(-x(m))*(besslk(0, sqrt(x(m)^2 + z0bar(m)^2))) + ((x(m)*besslk(1, sqrt(x(m)^2 + z0bar(m)^2)))/(sqrt(x(m)^2 + z0bar(m)^2)));

% Dimensional Cooling Rate
CR(m) = (((rho*c*(v^2)*alpha*tmpLP(i))/(2*pi*(k^2)*b))* abs(NCR(m)));
```

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ThermX(m) = \(-\exp(-x(m)) \ast ((\text{besselk}(0, \sqrt{x(m)^2 + z0bar(m)^2})) + ((x(m) \ast \text{besselk}(1, \sqrt{x(m)^2 + z0bar(m)^2}))) / (\sqrt{x(m)^2 + z0bar(m)^2}));

ThermZ(m) = ((\exp(-x(m)) \ast z0bar(m) \ast \text{besselk}(1, \sqrt{x(m)^2 + z0bar(m)^2})) / (\sqrt{x(m)^2 + z0bar(m)^2}));

% Non-dimensional Thermal Gradient
NTG(m) = \sqrt{(\text{ThermX}(m)^2 + \text{ThermZ}(m)^2)};

% Dimensional Thermal Gradient
G(m) = (((\rho \ast c \ast v \ast \alpha \ast \text{tmpLP}(i)) / (2 \ast \pi \ast (k^2) \ast b)) \ast \text{NTG}(m));

NR(m) = (\text{abs}(\text{NCR}(m)) / \text{abs}(\text{NTG}(m)));

x0bar(m+1) = x(m);

z0(m) = z0bar(m)/ND;

m = m + 1;

n = n + 1;

end

TempDepth(:,i)=z0bar ';
TempTmbar(:,i) = Tmbar ';
TempG(:,i)= \text{abs}(G');
TempCR(:,i)= \text{abs}(CR')

end

for p=1:(size(tmpLP))
   k=1;
   for j=1:200:a
      Depth(k,p)= TempDepth(j,p);
      FCR(k,p)= TempCR(j,p);
      FG(k,p) = TempG(j,p);
      k=k+1;
   end
end
B Matlab Code Listings for 3-D Rosenthal Solution

Listing B.1: Matlab File for Finding Roots (Melt Pool Dimensions)

```matlab
clc
clear all

% Value of Tmbar
Tmbar = input('Please input the value of Tmbar =');

% Initial guess for root finding
x0bar(1) = input('Please input the initial guess for root finding =');

% Resolution
a = input('Please input the resolution through the depth of the melt pool =');

% Normalized melt pool depth
ND = input('Please input the Normalized Melt pool depth =');

% Variance of Normalized melt pool length (0 < d < L)
d = linspace(0, ND, a);

D = d';

% Initializations
i = 1;
m = 1;

while n <= a

    z0bar(m) = D(m);

    y0bar(m) = 0;

    x(m) = fzero (@f, x0bar(m), [], Tmbar, y0bar(m), z0bar(m));

    cterm1(m) = ((exp(-(x(m) + sqrt(x(m)^2 + y0bar(m)^2 + z0bar(m)^2))))/(sqrt(x(m)^2 + y0bar(m)^2 + z0bar(m)^2)));

    bcterm1(m) = (x(m)/sqrt(x(m)^2 + y0bar(m)^2 + z0bar(m)^2));

    bcterm2(m) = (x(m)/(x(m)^2 + y0bar(m)^2 + z0bar(m)^2));

    NCR(m) = abs(0.5 * cterm1(m) * (1 + bcterm1(m) + bcterm2(m)));

end
```

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\[ x_{\bar{0}}(m+1) = x(m); \]
\[ z_{0}(m) = z_{0\bar{0}}(m)/ND; \]
\[ m = m + 1; \]
\[ n = n + 1; \]
\end

Listing B.2: Matlab File for Equation Call

```matlab
function value = f(x0bar, Tmbar, y0bar, z0bar)
    value = Tmbar - 0.5 * ((exp(-(x0bar + sqrt(x0bar^2 + y0bar^2 + z0bar^2))))/ (sqrt(x0bar^2 + y0bar^2 + z0bar^2)));
```
C  Matlab Code Listings for 2-D Uniform Distributed Case

Listing C.1: Matlab Program for Finding Roots (Melt Pool Dimensions)

```matlab
clc

clear all

% Value of Tmbar
Tmbar = input('Please input the value of Tmbar = ');

% Initial guess for root finding
x0bar(1) = input('Please input the initial guess for root finding = ');

% Resolution
a = input('Please input the resolution through the depth of the melt pool = ');

% Normalized melt pool depth
ND = input('Please input the melt pool depth = ');

d = linspace(0 ,ND,a);
D = d';

% Initializations
m = 1;
n = 1;

% Total width of the laser
wbar = input('Please input the beam width = ');

% For integrating the point source solution between -wbar/2 to wbar/2
wbar2 = wbar/2;

tmpCR = [];
tmpGradX = [];
tmpGradZ = [];

while n <= a
    z0bar(m) = D(m);
    x(m) = fzero(@(f,x0bar(m),[],Tmbar,z0bar(m),wbar2);
```

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```matlab
save ('temp1', mat')
tmpCR = quadl (@mycool, -1, 1, [], [], x(m), z0bar(m), wbar2);
tmpGradX = quadl (@myGradX, -1, 1, [], [], x(m), z0bar(m), wbar2);
tmpGradZ = quadl (@myGradZ, -1, 1, [], [], x(m), z0bar(m), wbar2);
NCR(m) = abs(tmpCR);
GX(m) = tmpGradX;
GZ(m) = tmpGradZ;
TG(m) = sqrt((GX(m)^2 + (GZ(m)^2));
x0bar(m+1) = x(m);
z0(m) = z0bar(m)/ND;
m = m + 1;
n = n + 1;
end
```

Listing C.2: Matlab Function File for Equation Call

```matlab
function ExpValue = f(x0bar, Tmbar, z0bar, wbar2)
tmp = quadl (@myfun, -1, 1, [], [], x0bar, z0bar, wbar2);
ExpValue = Tmbar - tmp;
```

Listing C.3: Matlab Function File for Numerical Integration to Find the Roots

```matlab
function [ value ] = myfun(u, x0barm, z0barm, wbar2);
value = 0.5 * (exp(-(x0barm - u*wbar2)) * besselk(0, sqrt((x0barm - u*wbar2)^2 + (z0barm)^2)));
```

Listing C.4: Matlab Function File for Evaluating Solidification Cooling rate

```matlab
function [ CRate ] = mycool(u, x0bar, z0bar, wbar2);
CRate = 0.5 * exp(-(x0bar - u*wbar2)) * (besselk(0, sqrt((x0bar - u*wbar2)^2 + z0bar^2)) + ( (x0bar - u*wbar2)/sqrt((x0bar - u*wbar2)^2 + z0bar^2)) * besselk(1, sqrt((x0bar - u*wbar2)^2 + z0bar^2))) ;
```

Listing C.5: Matlab Function File for Evaluating X-Component of Thermal Gradient

```matlab
function [ GradX ] = myGradX(u, x0bar, z0bar, wbar2);
GradX = -0.5 * exp(-(x0bar - u*wbar2)) * (besselk(0, sqrt((x0bar - u*wbar2)^2 + z0bar^2)) + ( (x0bar - u*wbar2)/sqrt((x0bar - u*wbar2)^2 + z0bar^2)) * besselk(1, sqrt((x0bar - u*wbar2)^2 + z0bar^2))) ;
```
Listing C.6: Matlab Function File for Evaluating Y-Component of Thermal Gradient

```matlab
function [GradZ] = myGradZ(u, x0bar, z0bar, wbar2);
GradZ = -0.5 * exp(-(x0bar-u+wbar2)).* (z0bar.^sqrt((x0bar-u+wbar2).^2+z0bar^2)) .* besseldk(1, sqrt((x0bar-u+wbar2).^2+z0bar^2));
```

Listing C.7: Matlab Program for Evaluating Normalized and Actual Cooling Rates and Thermal Gradients

```matlab
clc
clear all
% Definition of constants
rho = input('Please input the value of mass density =');
c = input('Please input the value of specific heat =');
k = input('Please input the value of thermal conductivity =');
v = input('Please input the value of velocity =');
b = input('Please input the value of thickness of the wall =');
Tm = input('Please input the value of melting temperature =');
T0 = input('Please input the value of initial temperature =');
alpha = 0.35;  % Fraction of the absorbed laser power
wbar = input('Please input the value of beam width =');
wbar2 = wbar/2;  % For integration purposes, the center of the laser is chosen as the origin and hence the integration is from -wbar/2 to wbar/2
tmpLP = input('Please input the value of laser power =');
tmpx0bar = input('Please input the initial guess for rootfinding =');
tmpnd = input('Please input the melt pool depth value =');
for i=1:size(tmpLP)
Tmbar = ((pi*k*b*(Tm - T0))/(alpha*tmpLP(i)));
x0bar(i) = tmpx0bar(i)
% Resolution
a = input('Please input the resolution through the depth of the melt pool =');
ND = tmpnd(i)
% Variance of Normalized melt pool depth (0 < d < L)
d = linspace(0,ND,a);
D = d';
% Initializations
m = 1;
```

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while n <= a
    z0bar(m) = D(m);
    x(m) = fzero (@f, x0bar(m), [], Tmbar, z0bar(m), wbar2);
    % Non-dimensional Cooling Rate
    tmpCR = quadl (@mycool, -1,1, [], x(m), z0bar(m), wbar2);
    NCR(m) = abs(tmpCR);
    % Dimensional Cooling Rate
    CR(m) = (((rho*c*(V^2)*alpha*tmpLP(i))/(2*pi*(k^2)*b))* abs(NCR(m)));
    % Thermal Gradient in the x-direction
    tmpGradX = quadl (@myGradX, -1,1, [], x(m), z0bar(m), wbar2);
    GX(m) = tmpGradX;
    % Thermal Gradient in the Z-direction
    tmpGradZ = quadl (@myGradZ, -1,1, [], x(m), z0bar(m), wbar2);
    GZ(m) = tmpGradZ;
    % Non-dimensional Thermal Gradient
    NTG(m) = sqrt((GX(m))^2 + (GZ(m))^2);
    % Dimensional Thermal Gradient
    G(m) = (((rho*c*v*alpha*tmpLP(i))/(2*pi*(k^2)*b))* NTG(m));
    x0bar(m+1) = x(m);
    z0(m) = z0bar(m)/ND;
    m = m + 1;
    n = n + 1;
end
TempDepth(:,i) = z0bar';
Tempz0(:,i) = z0';
TempTmbar(:,i) = Tmbar';
NtempCR(:,i) = abs(NCR');
NtempNTG(:,i) = abs(NTG');
TempG(:,i) = abs(G');
TempCR(:,i) = abs(CR');
end
for p = 1: (size(tmpLP))
    k = 1;
    for j = 1:500:

Depth(k, p) = TempDepth(j, p);
NDepth(k, p) = Tempz0(j, p);
NFCR(k, p) = NtempCR(j, p);
NFG(k, p) = NtempNTG(j, p);
FCR(k, p) = TempCR(j, p);
FG(k, p) = TempG(j, p);
k = k + 1;
end
end
D Matlab Code Listings for 3-D Uniform Distributed Case with Circular Beam Profile

Listing D.1: Matlab File for Finding Roots (Melt Pool Dimensions)

```matlab
clc
clear all
close all

% Value of Tmbar
Tmbar = input('Please input the value of Tmbar = ');

% Initial guess for root finding
x0bar = input('Please input the initial guess for root finding = ');

% Resolution
a = input('Please input the resolution through the depth of the melt pool = ');

% Normalized melt pool depth
ND = input('Please input the melt pool depth = ');
d = linspace(0,ND,a);
D = d';

% Initializations
m = 1;
n = 1;

% Total width of the laser
wbar = input('Please input the value of beam width = ');

% For integrating the point source solution between -wbar/2 to wbar/2
wbar2 = wbar/2;
tmpCR = [];

while n <= a
    z0bar(m) = D(m);
    y0bar(m) = 0;
    x(m) = fzero(@(x,x0bar(m),[],Tmbar,y0bar(m),z0bar(m),wbar2);
    tmpCR = dblquad(@(y,x,y0bar(m),z0bar(m),wbar2);
end
```
tmpGradX = dblquad (@myGradX, -1, 1, -1, 1, [], [], x(m), y0bar(m), z0bar(m), wbar2);

tmpGradY = dblquad (@myGradY, -1, 1, -1, 1, [], [], x(m), y0bar(m), z0bar(m), wbar2);

tmpGradZ = dblquad (@myGradZ, -1, 1, -1, 1, [], [], x(m), y0bar(m), z0bar(m), wbar2);

NCR(m) = tmpCR;

GX(m) = tmpGradX;

GY(m) = tmpGradY;

GZ(m) = tmpGradZ;

NTG(m) = sqrt((GX(m)^2 + (GY(m))^2 + (GZ(m))^2));

x0bar(m+1) = x(m);

m = m + 1;

n = n + 1;

end

Listing D.2: Matlab File for Equation Call

function [ExpValue] = f(x0bar, Tmbar, y0bar, z0bar, wbar2)

tmp = dblquad (@myfun, -1, 1, -1, 1, [], [], x0bar, y0bar, z0bar, wbar2);

ExpValue = Tmbar - tmp;

Listing D.3: Matlab File for Numerical Integration to Find the Roots

% Circular Beam (Numerical Integration for Root Finding)

function [value] = myfun(u, v, x0bar, y0bar, z0bar, wbar2);

num = exp(-((x0bar - (((v+1)*2*wbar2/4)*cos(pi*(u+1)))) + sqrt((x0bar - (((v+1)*2*wbar2/4)*cos(pi*(u+1)))),^2 + (y0bar - (((v+1)*2*wbar2/4)*sin(pi*(u+1)))),^2 + z0bar.^2));

den = sqrt((x0bar - (((v+1)*2*wbar2/4)*cos(pi*(u+1)))),^2 + (y0bar - (((v+1)*2*wbar2/4)*sin(pi*(u+1)))),^2 + z0bar.^2);

value = 0.125*(v+1).*(num./den);

Listing D.4: Matlab Function File for Evaluating Solidification Cooling rate

% Dimensionless Cooling Rate Expression for a Circular Laser Beam

function [CRate] = mycool(u, v, xm, y0bar, z0bar, wbar2);

num = exp(-((xm - (((v+1)*2*wbar2/4)*cos(pi*(u+1)))) + sqrt((xm - (((v+1)*2*wbar2/4)*cos(pi*(u+1)))),^2 + (y0bar - (((v+1)*2*wbar2/4)*sin(pi*(u+1)))),^2 + z0bar.^2));
\[ \text{den} = \sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}; \]

\[ \text{cterm1} = \frac{\text{num}}{\text{den}}; \]

\[ \text{bcterm1} = \frac{(x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))}{\sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}}; \]

\[ \text{bcterm2} = \frac{(x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))}{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}}; \]

\[ \text{CRate} = \text{abs}(0.125 \cdot (v+1) \cdot \text{cterm1} \cdot (1 + \text{bcterm1} + \text{bcterm2})]; \]

### Listing D.5: Matlab Function File for Evaluating X-Component of Thermal Gradient

```matlab
% Expression for X-component of Dimensionless Thermal Gradient (Circular Laser Beam)

function [GradX] = myGradX(u, v, x_m, y0bar, z0bar, wbar2);

num = \exp((-((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1)))) + \sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}});

den = \sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}};

cterm1 = \frac{\text{num}}{\text{den}};

bcterm1 = \frac{(x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))}{\sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}};

bcterm2 = \frac{(x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))}{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}};

GradX = \text{abs}(-0.125 \cdot \text{cterm1} \cdot (1 + \text{bcterm1} + \text{bcterm2})];
```

### Listing D.6: Matlab Function File for Evaluating Y-Component of Thermal Gradient

```matlab
% Expression for X-component of Dimensionless Thermal Gradient (Circular Laser Beam)

function [GradY] = myGradY(u, v, x_m, y0bar, z0bar, wbar2);

num = \exp((-((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1)))) + \sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}});

den = \sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}};

cterm2 = \frac{\text{num}}{\text{den}};

bcterm3 = \frac{1}{\sqrt{((x_m - ((v+1) \cdot 2 + wbar2/4) \cdot \cos (\pi \cdot (u+1))))^2 + (ybar - (((v+1) \cdot 2 + wbar2/4) \cdot \sin (\pi \cdot (u+1))))^2 + z0bar \cdot \text{^2}}});
```
Listing D.7: Matlab Function File for Evaluating Z-Component of Thermal Gradient

% Expression for X-component of Dimensionless Thermal Gradient (Circular Laser Beam)

function [GradZ] = myGradZ(u, v, x0bar, z0bar, wbar2);
num = exp(-(x - ((v+1)*2*wbar2/4)*cos(pi*(u+1)))) + sqrt((x - ((v+1)*2*wbar2/4)*cos(pi*(u+1)))^2 + (y - ((v+1)*2*wbar2/4)*sin(pi*(u+1)))^2 + z0bar^2);
den = (x - ((v+1)*2*wbar2/4)*cos(pi*(u+1)))^2 + (y - ((v+1)*2*wbar2/4)*sin(pi*(u+1)))^2 + z0bar^2);
cterm2 = (num./den);
bcterm4 = 1./sqrt((x - ((v+1)*2*wbar2/4)*cos(pi*(u+1)))^2 + (y - ((v+1)*2*wbar2/4)*sin(pi*(u+1)))^2 + z0bar^2);
GradZ = abs(-0.125*(u+1)*z0bar.*cterm2.*(1+bcterm4));

Listing D.8: Matlab Function File for Evaluating Normalized and Actual Cooling Rates and Thermal Gradients

clear all
% Definition of constants
rho = input('Please input the value of mass density ');
c = input('Please input the value of specific heat ');
k = input('Please input the value of thermal conductivity ');
v = input('Please input the value of velocity ');
Tm = input('Please input the value of melting temperature ');
T0 = input('Please input the value of initial temperature ');
alpha = 0.35; % Fraction of the absorbed laser power
wbar = input('Please input the value of beam width ');
wbar2 = wbar/2; % For integration purposes, the center of the laser is chosen as the origin and hence the integration is from -wbar/2 to wbar/2

tmpLP = input('Please input the value of laser power ');
tmpx0bar = input('Please input the initial guess for root finding ');
tmpnd = input('Please input the melt pool depth value ');
for i=1:size(tmpLP)
    Tmbar = ((2*pi*k^2*(Tm-T0))/(rho*c*v*alpha*tmpLP(i)));
\[
x_{0\text{bar}}(1) = \text{tmp}x_{0\text{bar}}(i)
\]
\[
\% \text{ Resolution}
\%
\]
\[
a = \text{input}(\text{'}\text{Please input the resolution through the depth of the melt pool}\text{'});
\]
\[
\% \text{ Normalized melt pool depth}
\% \text{ Variance of Normalized melt pool length (0 < d < L)}
\]
\[
\text{ND} = \text{tmpnd}(i);
\]
\[
d = \text{linspace}(0, \text{ND}, a);
\]
\[
\text{D} = \text{d}';
\]
\[
\% \text{ Initializations}
\]
\[
t = 1;
\]
\[
m = 1;
\]
\[
n = 1;
\]
\[
\text{while } n \leq a
\]
\[
\quad z_{0\text{bar}}(m) = \text{D}(m);
\]
\[
\quad y_{0\text{bar}}(m) = 0;
\]
\[
\quad x(m) = \text{fzero}(\text{at}, x_{0\text{bar}}(m), [], \text{Tmbar}, y_{0\text{bar}}(m), z_{0\text{bar}}(m), \text{wbar2});
\]
\[
\% \text{ Non-dimensional Cooling Rate}
\]
\[
\text{tmpCR} = \text{dblquad}(\text{atmycool}, -1, 1, -1, 1, [], [], x(m), y_{0\text{bar}}(m), z_{0\text{bar}}(m), \text{wbar2});
\]
\[
\text{NCR}(m) = \text{abs}(\text{tmpCR});
\]
\[
\% \text{ Dimensional Cooling Rate}
\]
\[
\text{CR}(m) = (((\text{rho} \ast \text{c} \ast \text{v}) / (2 \ast \text{k}))^2) \ast ((\text{alpha} \ast \text{tmpLP}(i) \ast \text{v}) / (\pi \ast \text{k})) \ast \text{NCR}(m);
\]
\[
\% \text{ Thermal Gradient in the x-direction}
\]
\[
\text{tmpGradX} = \text{dblquad}(\text{atmyGradX}, -1, 1, -1, 1, [], [], x(m), y_{0\text{bar}}(m), z_{0\text{bar}}(m), \text{wbar2});
\]
\[
\text{GX}(m) = \text{tmpGradX};
\]
\[
\% \text{ Thermal Gradient in the Y-direction}
\]
\[
\text{tmpGradY} = \text{dblquad}(\text{atmyGradY}, -1, 1, -1, 1, [], [], x(m), y_{0\text{bar}}(m), z_{0\text{bar}}(m), \text{wbar2});
\]
\[
\text{GY}(m) = \text{tmpGradY};
\]
\[
\% \text{ Thermal Gradient in the Z-direction}
\]
\[
\text{tmpGradZ} = \text{dblquad}(\text{atmyGradZ}, -1, 1, -1, 1, [], [], x(m), y_{0\text{bar}}(m), z_{0\text{bar}}(m), \text{wbar2});
\]
\[
\text{GZ}(m) = \text{tmpGradZ};
\]
\[
\% \text{ Non-dimensional Thermal Gradient}
\]
\[
\text{NTG}(m) = \text{sqrt}(((\text{GX}(m))^2 + (\text{GY}(m))^2 + (\text{GZ}(m))^2));
\]
\[
\% \text{ Dimensional Thermal Gradient}
\]
\[
\text{G}(m) = (((\text{rho} \ast \text{c} \ast \text{v}) / (2 \ast \text{k}))^2) \ast ((\text{alpha} \ast \text{tmpLP}(i)) / (\pi \ast \text{k})) \ast \text{NTG}(m);
\]
\[
\text{x}_{0\text{bar}}(m+1) = x(m);
\]
\[ z_0(m) = \frac{z_{0\text{bar}}(m)}{N\text{D}}; \]

\[ m = m + 1; \]

\[ n = n + 1; \]

end

TempDepth(:, i) = \text{z}_{0\text{bar}}' ;

Tempz0(:, i) = \text{z0}' ;

TempTmbar(:, i) = \text{Tmbar}' ;

NtempCR(:, i) = abs(NCR') ;

NtempNTG(:, i) = abs(NTG') ;

TempG(:, i) = abs(G') ;

TempCR(:, i) = abs(CR') ;

end

for p = 1: \text{size (tmpLP)}

\[ k = 1; \]

\[ \text{for } j = 1:500;a \]

\[ \text{Depth}(k, p) = \text{TempDepth}(j, p); \]

\[ \text{NDepth}(k, p) = \text{Tempz0}(j, p); \]

\[ \text{NCR}(k, p) = \text{NtempCR}(j, p); \]

\[ \text{NTG}(k, p) = \text{NtempNTG}(j, p); \]

\[ \text{FCR}(k, p) = \text{TempCR}(j, p); \]

\[ \text{FG}(k, p) = \text{TempG}(j, p); \]

\[ k = k + 1; \]

end

end
E Matlab Code Listings for 3-D Uniform Distributed Case with Square Beam Profile

Listing E.1: Matlab File for Finding Roots (Melt Pool Dimensions)

```matlab
clc
clear all
close all

% Value of Tmbar
Tmbar = input('Please input the value of Tmbar = '); % Value of Tmbar

% Initial guess for root finding
x0bar = input('Please input the initial guess for root finding = '); % Initial guess for root finding

% Resolution
a = input('Please input the resolution through the depth of the melt pool = '); % Resolution

% Normalized melt pool depth
ND = input('Please input the melt pool depth = '); % Melt pool depth

d = linspace(0, ND, a); % Melt pool depth
D = d';

% Initializations
m = 1;
n = 1;

% Total width of the laser
wbar = input('Please input the value of beam width = '); % Laser beam width

% For integrating the point source solution between -wbar/2 to wbar/2
wbar2 = wbar/2;

[tmpCR] = [];

while n <= a
    z0bar(m) = D(m);
end
```
Listing E.2: Matlab File for Equation Call

function [ExpValue] = f(x0bar, Tmbar, y0bar, z0bar, wbar2)

    tmp = dblquad(@(u,v,x0bar,y0bar,z0bar,wbar2), -1, 1, -1, 1, x0bar, y0bar, z0bar, wbar2);
    ExpValue = Tmbar - tmp;

Listing E.3: Matlab File for Numerical Integration to Find the Roots

function [value] = myfun(u,v,x0bar,y0bar,z0bar,wbar2);

    num = exp(-((x0bar-(u*wbar2))^2 + (y0bar-(v*wbar2))^2 + z0bar^2));
    den = 8*(sqrt((x0bar-(u*wbar2))^2 + (y0bar-(v*wbar2))^2 + z0bar^2));
    value = (num./den);

Listing E.4: Matlab Function File for Evaluating Solidification Cooling rate

function [CRate] = mycool(u,v,x0bar,y0bar,z0bar,wbar2);

% Expression for Dimensionless Cooling Rate (Square Laser Beam)
cterm1 = \((\exp(-((x_m-u*\bar{w}2) + \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)})^2)) / (\sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)}))\);

bcterm1 = ((x_m-u*\bar{w}2) / \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)});

bcterm2 = ((x_m-u*\bar{w}2) / ((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2));

CRate = \text{abs}(0.125 * cterm1 .* (1 + bcterm1 + bcterm2));

Listing E.5: Matlab Function File for Evaluating X-Component of Thermal Gradient

function [GradX] = myGradX(u, v, x0bar, z0bar, wbar2);

cterm1 = \((\exp(-((x_m-u*\bar{w}2) + \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)})^2)) / (\sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)}))\);

bcterm1 = ((x_m-u*\bar{w}2) / \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)});

bcterm2 = ((x_m-u*\bar{w}2) / ((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2));

GradX = \text{abs}(-0.125 * cterm1 .* (1 + bcterm1 + bcterm2));

Listing E.6: Matlab Function File for Evaluating Y-Component of Thermal Gradient

function [GradY] = myGradY(u, v, x0bar, z0bar, wbar2);

cterm2 = \((\exp(-((x_m-u*\bar{w}2) + \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)})^2)) / (\sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)}))\);

bcterm3 = 1 / \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)});

GradY = \text{abs}(-0.125 * (y_0-bar-v*\bar{w}2) .* cterm2 * (1 + bcterm3));

Listing E.7: Matlab Function File for Evaluating Z-Component of Thermal Gradient

function [GradZ] = myGradZ(u, v, x0bar, z0bar, wbar2);

cterm2 = \((\exp(-((x_m-u*\bar{w}2) + \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)})^2)) / (\sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)}))\);

bcterm4 = 1 / \sqrt{((x_m-u*\bar{w}2)^2+(y_0-bar-v*\bar{w}2)^2+z_0-bar.2^2)});

GradZ = \text{abs}(-0.125 * z_0-bar.* cterm2.*(1 + bcterm4));
Bibliography


[67] S. Kelly and S. Kampe, “Microstructural Evolution in Laser-Deposited Multi-layer Ti-6Al-


