A Framework to Link Localized Cooling and Properties of Directed Energy Deposition (DED)-Processed Ti-6Al-4V

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Abstract

Additive manufacturing (AM) of titanium alloys is a rapidly growing field due to an increase in design flexibility of parts. However, AM parts are highly anisotropic in material microstructure and mechanical behavior due to the change of the local processing conditions in the build-up process. This study follows a link chain model to investigate the relationships between process parameters, cooling rate, porosity and mechanical behavior. **The aim of this work is to present a framework that is inspired by the three-link chain model. The framework combines theoretical, computational and experimental approaches. We demonstrate this by using an in-house thermal simulator to link predicted cooling rates with micrographs describing experimental shape descriptors to develop a relationship between solidification cooling rate and porosity geometry.** Finally, representative volume elements from predicted porosity maps allow for a prediction of mechanical properties at localized areas. The capability of being able to predict mechanical behavior of titanium alloys is demonstrated for the directed energy deposition process.

Keywords: Directed Energy Deposition (DED), cooling rate, anisotropy, porosity, titanium alloys

1. Introduction

The motivation for this study is fueled by the growing ubiquity of additive manufacturing (AM) for customized and complex parts in a wide variety of industries, especially biomedical and aerospace. In particular, additively manufactured titanium alloys, such as Ti-6Al-4V, have seen an increase in demand because they possess high strength, are light weight, and have increased ductility [1]. However, a major challenge of AM is the anisotropy of as-built components due to the differences in cooling rate during the process and the resulting material microstructure. Before a prediction of the global properties of an AM part can

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be accomplished, an understanding of the localized properties is required to predict and control areas that could potentially lead to defects. Predicting the “weakest links” of an AM component is essential to ensure that quality standards are met [2]. Figure 1 shows the three-link chain model that drives the localized analysis in this study and follows the general concept of processing-structure-properties-performance, presented in [3], but with differences in the specific relationships. Here, the links are identified as *process parameters* influencing the *local cooling rate*, which influences the *local porosity* within an AM component, and in turn influences *local mechanical behavior*. This study considers each link individually to determine a broad framework that evaluates material performance via a combination of experimental and computational methods.

Figure 1: Three-link chain model that is the underlying method for the localized analysis.

1.1. Directed energy deposition (DED) and porosity

Directed energy deposition (DED) is a class of AM processes that implements a focused thermal energy source, such as a laser, to melt deposited material [4]. DED processes are mostly electron beam and laser based methods. Laser-based DED has multiple names that describe the same process, including Directed Light Fabrication (DLF), Direct Metal Deposition (DMD), 3D Laser Cladding, Laser-Based Metal Deposition (LBMD), Laser Freeform Fabrication and Laser Engineered Net Shaping (LENS) [4]. This study focuses on LENS, in which the focal point of metallic powder deposition is aligned with the laser’s focal point, allowing the powders to fuse together within a melt pool that moves with the aligned beam [5]. Translation of the build platform or the laser optic in the Z-direction allows an additional layer to fuse with the layer beneath. Among the many variables and parameters in LENS, laser power, scan speed, powder flow rate, hatch spacing and layer thickness have the greatest influence on final material properties. As seen in Fig. 2, hatch spacing is the bead overlap within a layer, and layer thickness is the Z translation of the laser-powder focal point. Slight changes in process parameters can lead to drastic changes in microstructure and mechanical behavior of the final component [6].

Figure 2: Schematic of the laser engineered net shaping (LENS) process where the X axis is the hatch direction, the Y axis is the scan direction and the Z axis is the build direction.

Several studies illustrate the influence process parameters have on microstructure, especially porosity formation. Two categories of porosity appear during DED processes due to the non-uniform heat transfer **during** the process: interlayer and intralayer porosity [7]. Porosity due to the lack of fusion is interlayer porosity at the interfaces between each layer of melted powder [8]. This is a result of the discrepancy in temperature distribution within the melt pool, including the unwanted presence of un-melted powder particles that flow to the underlying, colder layers [8]. Intralayer porosity is a result of vaporization at the melt pool, which can entrap gas, such as oxides, into the component [9]. X-ray computed tomography has demonstrated the presence of interlayer and intralayer porosity in DED-processed stainless steel and titanium alloys and that altering process parameters influence the size, shape and distribution of the pores, especially interlayer pores [9]. The size and shape of these pores are anisotropic due to the subsequent layers of material re-melting and the surfaces of a component undergoing more convection and radiation of heat [10]. Interlayer porosity due to lack of fusion of powders between layers leads to strength anisotropy that is dependent on relative orientation to the build and scan directions, with yield strengths in the X and Y (scan) directions higher than that in the Z (build) direction [10]. Literature illustrates that there is a relationship between porosity and global energy density (GED) where interlayer porosity is found at the low extreme of GED values and intralayer porosity is found at the high extreme of GED values for a given process and material[11], as seen in Fig. 3. GED can be defined as a combination of several process parameters [12]:

$$GED = \frac{P}{sd} \quad (1)$$

where P is the output laser power in watts, s is the scan speed in millimeters per second, and d is the laser beam diameter in millimeters.

Figure 3: Relationship between porosity and global energy density in DED processes.

1.2. Solidification cooling rate and porosity prediction

It is our hypothesis that different solidification cooling rates during a DED build of a Ti-6Al-4V component lead to various porosity distributions. For example, the extensive and ordered porosity in the build direction versus the porosity in the scan direction results in anisotropic mechanical behavior due to insufficient fusion and rapid cooling between layers [13]. Porosity formation due to solidification during casting of Al-4.5 pct. Cu plates was mathematically modeled using shape descriptors of radius of pore and area fraction [14]. A comprehensive study of the influence of cooling rate on pore diameter, area fraction of pores, microstructure and mechanical properties were completed for cast LM13 alloy and demonstrated that increasing cooling rate decreased porosity area fraction and size as well as improved mechanical properties [15]. However, DED-processed materials have cooling rates that range from 102 to 104 K/s and cast materials have cooling rates that range from 1 to 100 K/s [16]. The anisotropy in tensile behavior of DED-processed, wrought and cast Ti-6Al-4V is influenced by the interlayer porosity due to crack initiation at pore sites as opposed to intralayer porosity [13] and has shown to depend on the orientation of the build and the location of a specimen relative to the substrate [17]. In summary, previous studies have shown that DED-processed Ti-6Al-4V components exhibit porosity and strength anisotropy.

Recent modeling efforts in electron beam additive manufacturing evaluates the thermal evolution of the melt pool of a powder bed fused part with varying initial porosity levels [18]. Several studies have predicted microstructural characteristics, such as dendritic spacing of stainless steel alloys, using cooling rate [10, 11, 13, 19]. Evaluating porosity in a DED-processed component is a simple method to evaluate a microstructural characteristic and its link with cooling. This forms the crux of the proposed framework that demonstrates the relationships between cooling and porosity.

1.3. Objective

This paper aims to propose a framework to demonstrate the influence of the solidification cooling rate on strength and porosity anisotropy. Recent studies in AM lack more descriptive pore characteristics while investigating the relationships between process parameters and mechanical properties. Linking process parameters and mechanical properties emphasizes the need for an understanding of localized properties because of the high variability and anisotropy of a DED-processed component. The proposed framework couples

computational simulations with experimental results to predict localized porosity and mechanical properties, aiming to establish the relationship between cooling rate and pore shape descriptors.

2. Experimental Methods

2.1. DED-processed Ti-6Al-4V cubic components

A Laser Engineered Net Shaping system in the Quad City Manufacturing Laboratory in Rock Island, IL built three Ti-6Al-4V 40 mm x 40 mm x 40 mm cubic components. The DED process utilized a 1 kW Ytterbium continuous wave (CW), Gaussian profile, fiber optic laser coupled with inert shield gas in an enclosed environment and four-axis capability. Four coaxial nozzles surrounded the laser beam optic and deposited Ti-6Al-4V powders with a size distribution from 45 to 150 μm in diameter.

Each Ti-6Al-4V component was built separately on an unheated Ti-6Al-4V substrate plate within the DED enclosure with the process parameters outlined in Table 1. The tool path alternated between a laser on the ON mode during a scan at 0 and 180 degrees between beads within each layer and on the OFF mode while moving the laser optic in the build direction, or the positive Z direction by the layer thickness. Figure 2 illustrates the coordinate system of the DED system, the hatch spacing and tool path in the specified reference frame.

Table 1: Process parameters of each Ti-6Al-4V cubic component.

Output Laser Power	Scan Speed	Beam Diameter	Powder Feed Rate	Hatch Spacing	Layer Thickness
710 W					
800 W	10 mm/s	1.83 mm	0.12 g/s	1.25 mm	0.95 mm
940 W					

2.2. Global analysis of DED-processed components

A method based on the generalized mixed rule (GMR) [20] had been used to globally define and predict for porosity throughout a component by implementing three sets of process parameters with varying laser power values [21]. However, a GMR-based method evaluates the average porosity and tensile behavior of an entire component at three orientations although the porosity and strength can vary within an orientation of the component, depending on the distance from the surface of the component as shown in our previous work [21].

The global analysis conducted in this study focuses on the component processed with a laser power of 800 W and how bulk porosity and mechanical properties vary with location and orientation of the tensile specimen. Mechanical behavior was determined by the uniaxial tensile test of specimens made from the cubic using the wire electrical discharge machining (wire-EDM). The Archimedes method determined the bulk volume porosity for

each specimen. The purpose of the global analysis is to illustrate the overall patterns of a component’s microstructure and mechanical behavior throughout the cube.

2.2.1. Tensile testing of machined DED specimens

Tensile specimens were machined by wire-EDM from each cubic component in three different orientations as defined in Fig. 4 and Table 2 . The dimensions of tensile specimens followed ASTM E8 standards [22] with a gauge length of 10.0 mm, gauge width of 2.5 mm, and thickness of 1.2 mm. Tensile specimens with orientation “A” were machined from the XZ plane at various depths in the Y direction. These “A” specimens were subject to a uniaxial tensile direction, or the principal load axis, in the build direction, the Z axis. Tensile specimens with orientation “B” were machined from the XY plane with a principal load axis in the X axis. Tensile specimens with orientation “C” were machined through the X direction on the XZ plane with a principal load axis in the scan direction, or Y axis.

Figure 4: The various orientations of the machined tensile specimens are defined as “A”, “B” and “C” and pertain to the DED coordinate system.

Table 2: Description of each orientation tested.

Orientation	Sample Plane	Unit vector normal to plane	Principal load axis
A	XZ	Y	Z
B	XY	Z	X
C	YZ	X	Y

In the 710 W-processed cubic component, four tensile specimens were machined in each orientation as illustrated in Fig. 4. Two specimens in the “A” orientation, four in the “B” orientation, and four in the “C” orientation were successfully tested under uniaxial load and measured for bulk porosity, resulting in ten data points. Some of the specimens exhibited substantial surface porosity and experienced premature deformation during pre-load, which was meant to relieve any compressive stresses while gripping the specimens [23]. However, the noticeable surface porosity resulted in crack initiation and bending before a complete uniaxial tensile test could be completed, as surface and subsurface porosity are the most

likely sites of crack initiation and premature deformation in Ti-6Al-4V [24]. Therefore, the data from these specimens do not represent uniaxial loading and were excluded. In the 800 W-processed cubic component, about eight to twelve tensile specimens were machined from each orientation. Ten specimens in the “A” orientation, seven in the “B” orientation, and ten in the “C” orientation were successfully tested under uniaxial load and measured for bulk porosity, resulting in 27 data points, with three specimens in the “B” orientation not successfully tested. In the 940 W-processed cubic component, eight tensile specimens in the “C” orientation were machined, successfully tested under uniaxial load and measured for bulk porosity. A total of 41 data points with mechanical test and porosity information were studied. The tension tests were performed on a servo-hydraulic machine with 100 kN load capacity at a strain rate of 0.25 mm/min. This quasi-static test utilized a 10 mm extensometer to measure strain.

2.2.2. Global porosity characterization

Porosity volume fraction and density were measured using the Archimedes method [25] for each of the three cubic components prior to machining and three times for each tensile specimen prior to tensile test for a total of 123 complete measurements. The specific type of Archimedes measurement used was the suspension technique. The resolution of the Archimedes method for each specimen was 0.001 g/mm^3 , with the volume of each specimen less than 50 mm^3 . The accuracy of this method has been demonstrated to be 0.03% for volumes less than 50 mm^3 , which is comparable to the accuracy of pycnometry, at 0.01% [26]. After failure, porosity and density were measured three times using the Archimedes method again for both halves of each tensile specimen. The mean values and standard deviations of porosity and density values for each tensile specimen were evaluated. Negligible differences of about 0.1% between the measurements before and after tensile tests were observed.

Compared to other density and porosity measurement methods for additive manufactured samples, the Archimedes method has demonstrated superior repeat accuracy of components with high density (i.e., above 95% density) and is the most reliable and cost effective method to measure the density of entire samples [25]. Note that the density of each sample examined in this paper is above 95%. The drawbacks of the Archimedes method include possible variations in measurements due to air bubbles that adhere to the surface of the sample and is exacerbated by increases in surface roughness [26]. In addition, the presence of surface porosity can introduce water to flow into the sample if they are not appropriately sealed, which would skew the density measurement [26]. The samples measured did not exhibit surface porosity. Surface roughness was not an issue because the samples were machined from the AM component using wire-EDM.

2.3. Localized analysis

Localized analysis of a DED-processed component addresses the challenges in establishing the global relationships between porosity and mechanical behavior of tensile specimens. The underlying method for the localized analysis in this study was the three-link chain model, as defined in the introduction [3]. Because solidification can lead to lack of fusion porosity due to thermal-dependent volume change at the melt pool, 2D micrographs of porosity

were analyzed at the probed points. Pore shape descriptors, including size, roundness, area fraction and nearest neighbor distance were shown to be dependent of solidification cooling rate. Subsequently, statistical relationships between the simulated cooling rate and the pore shape descriptors can generate representative porosity maps in a representative volume element (RVE), and therefore, RVEs in the finite element analysis can predict micro-mechanical behavior at localized areas of the DED-processed Ti-6Al-4V cubic component.

After preparing samples by cutting, mounting and polishing, 2D micrographs for image analysis of porosity size, shape and distribution were taken using optical microscopy. The evaluated cross-sections were cut from the tensile specimen grip area using an aluminum silica blade. The resolution of the 2D optical microscopy (OM) method was determined by the pixel size of the micrographs, which was $0.65\ \mu\text{m}$ by $0.65\ \mu\text{m}$. The accuracy of the 2D OM method by thresholding each individual micrograph is greater than that of an automatic global thresholding method where the same threshold cutoff value to identify pores is applied to all micrographs. In addition, the coefficient of variation of the 2D OM method is less than 0.1 mm/s with increasing accuracy with greater sample density [26]. The drawbacks of the 2D OM method includes potential inconsistency of imaging thresholding among various micrographs, micrographs are not representative of a sample and only capture two dimensions of porous structure, and cutting, polishing and etching the samples at many locations can become a time-consuming task.

Image analysis of 2D micrographs provided the area, roundness and nearest neighbor distance of each pore and the area fraction of pores in each micrograph, based on descriptor-based methodology for designing and predicting microstructure material systems for polymer nanocomposites [27]. Past work on polymer nanocomposites identified key descriptors of nanoparticles such as dispersion, geometry and composition and used the simulated annealing algorithm to reconstruct microstructure maps for finite element (FEA) analysis of mechanical behavior [27]. This paper identifies descriptors for pores in metallic alloys to reconstruct microstructure maps for FEA and takes this a step further to link the descriptors to processing conditions and solidification behavior.

3. Computational Methods

3.1. Thermal modeling and cooling rate

The thermal model captured the trend of the solidification rate throughout a unique DED build and matched with a numerical model that included convection at the melt pool [28]. In addition, experimental work that investigated the cooling rate during solidification of several DED-processed materials found that the relationship between the solidification rate and the melt pool length is a log-log trend, with an increase of solidification rate at lower melt pool lengths [29]. Increasing laser power has been shown to increase the length: width ratio of the melt pool during DED [30]. The proposed thermal model agreed with the trend of greater solidification rates at lower melt pool lengths in that the solidification rate decreased with increasing laser power from 710 to 940 W [28, 29, 30].

Process parameters were inputs into to an in-house simulation code that models any DED build as well as the melt pool and resulting residual stresses in a part [31]. One can output

the temperature history from any probed point within the built component. Each point underwent at least one cycle of solidification where the temperature cools from liquidus to solidus temperatures. Experimentally determined 2D micrographs of porosity distribution were also taken at these points to link the probed solidification cooling rates with porosity descriptors.

In this study, a thermodynamically consistent prediction of melt pool solidification served as a qualitative output of an in-house finite element software that takes process parameters, tool path, component geometry and the thermodynamic properties of Ti-6Al-4V as inputs [31]. The in-house code, named GAMMA code, demonstrates the evolution of the melt pool during a build. In this case, the model was a 40 mm by 40 mm by 40 mm Ti-6Al-4V with 212112 linear heat transfer hexahedral elements and 224315 nodes. Deposited powders onto the melt pool were approximated as solid clusters, where each element is approximated as a solid cluster and birthed during the deposition with the laser input. The laser input was approximated by a moving boundary flux, represented by the element degrees of freedom in the solution. The major benefit of the in-house code as opposed to a commercial software like ABAQUS is the drastic reduction (about 1000x) in computation time for a full part simulation. This is achieved through optimization of time-dependent boundary conditions and element birth routines based on the experimental tool path. A single-processor simulation of a build could take up to about six days for a commercial software, whereas the same simulation would take less than ten minutes for the in-house code.

The bottom of the base plate was fixed at 300K with convection and radiation boundary conditions applied everywhere else. The energy conservation equation was solved for the temperature distribution throughout the model. This equation has the following form:

$$\rho C_p^e(\theta) \frac{\partial \theta}{\partial t} = \nabla \cdot (k \nabla \theta) + q_{app}(\bar{x}, t) + q_{rad}(\theta) + q_{conv}(\theta) \quad (2)$$

where θ is the temperature, ρ is the material density, C_p^e is the effective heat capacity and k is the thermal conductivity. A moving Gaussian surface flux was used to model the laser, which is given by:

$$q_{app} = -\frac{2\eta P}{\pi R_{beam}^2} \exp(-2\frac{\bar{R}(\bar{x})^2}{R_{beam}^2}) \quad (3)$$

where η is the absorption coefficient of the material, P is the laser/electron beam power, R_{beam} is the beam radius, and $\bar{R}(\bar{x})$ is the radial distance from the heat source to the location of the material point of interest. Energy dissipation due to radiation effects q_{rad} was modeled by the following equation:

$$q_{rad} = \sigma \varepsilon [(\theta - \theta_0)^4 - (\theta_\infty - \theta_0)^4] \quad (4)$$

where σ is the Stefan-Boltzmann constant, ε is the emissivity of the material, θ_0 is the absolute zero temperature in Kelvins and θ_∞ is the ambient temperature. Energy dissipation due to convection (q_{conv}) **with the surrounding ambient temperature** were modeled by the following equation:

$$q_{conv} = h_{conv}(\theta - \theta_\infty) \quad (5)$$

where h_{conv} is the convection heat transfer coefficient. Lastly, the release of latent heat during solidification was modeled with the apparent heat capacity method [32]. The effective specific heat capacity C_p^e was modified based on the current temperature to capture latent heat effects:

$$C_p^e(\theta) = \begin{cases} C_p & \theta < \theta_S \\ C_p + \frac{\Delta H_L}{\theta_L - \theta_S} & \theta_S < \theta < \theta_L \\ C_p & \theta_L < \theta \end{cases} \quad (6)$$

where C_p is the material specific heat, ΔH_L is the change in enthalpy during the phase transition, θ_L is the liquidus temperature and θ_S is the solidus temperature. C_p can be treated as either a constant obtained from handbooks or as a temperature-dependent variable calculated from CALPHAD that takes various phases transformations into account. For the illustration of this three-link models, here, for simplicity, C_p is taken as a constant. Values used for various material properties and parameters are given in Table 3:

Table 3: Material and parameter values used for thermal model.

Name	Parameter/Property	Value
Convection heat transfer coefficient	h_{conv}	$0.00005 \frac{J}{mm^2 \cdot K}$
Emissivity	ε	0.2
Stefan-Boltzmann constant	σ	$5.6704 \times 10^{-14} \frac{W}{mm^2 \cdot K^4}$
Ambient temperature	θ_∞	300K
Processing power	P	710W
Beam radius	R_{beam}	800W
Heat capacity	C_p	940W
Density	ρ	0.915mm
Thermal conductivity	k	$0.6 \frac{J}{g \cdot K}$
Change in enthalpy	ΔH_L	$0.00799 \frac{g}{mm^3}$
Liquidus temperature	θ_L	$0.02 \frac{W}{mm \cdot K}$
Solidus temperature	θ_S	286 $\frac{J}{g}$
		1726.1K
		1607.4K

The thermal model does not consider convective effects that occur due to Marangoni forces, yielding predicted cooling rates that are larger than what is seen in experiments or in computational flow dynamics simulations. Previous studies show that these Marangoni convective cooling forces play a significant role in the cooling process for applications incorporating extreme thermal gradients such as welding [33, 34] and additive manufacturing [35, 36, 37]. Convective influence in the melt pool can be captured by implementing a reduced order model or by enlarging the conductivity to capture additional cooling. However, the goal of the current work is to present a preliminary but general framework that combines experimental and computational approaches to link process, structure and mechanical properties of additively manufacture parts. The resolution of the additional physics and a high fidelity localized analysis is out of scope of this general framework approach, though refining the resolution of the methods will be the primary focus of future work.

The solidification cooling rate for a location of the component was determined at the element of the computational model. Each element was 0.625 mm in width, 0.625 mm in length and 0.95 mm in height, with a volume of 0.371 mm³. The cooling rate of each location, or point of the component, was representative of this volume. The FEM process thermal model resulted in a temporal resolution of 0.001 seconds, which is high enough to capture the characteristic material properties to be experimentally examined and to capture the effect of Latent heat in solidification. This study assumed that the dominant influence during solidification occurred during the last re-melting cycle, as many areas of a component were prone to re-heating and re-melting during fusion of additional layers. As seen in the temperature profile in Fig. 7, there are two cycles of melting over time at the highlighted green element, with the last re-melting cycle as the circled region between the solidus and liquidus temperatures of Ti-6Al-4V. To calculate the solidification cooling rate at an individual probed point, the last re-melting cycle was evaluated between the liquidus and solidus boundaries of Ti-6Al-4V.

3.2. Representative volume element

Using the statistically determined relationships between the experimentally determined porosity shape descriptors and the simulated cooling rate calculation, 2D or 3D representative porosity maps can be generated. In this study, a 2D porosity map illustrated a case study for a solidification cooling rate of 750 K/s. Finite element analysis via ABAQUS meshed the porosity map with tetrahedral elements in 2D and an implemented Johnson-Cook damage model for Ti-6Al-4V [38] to illustrate how pores in the AM component **change shape and lead to shear bands in various orientations of tensile load**. The Johnson-Cook material parameters are listed in Table 4.

Table 4: Johnson-Cook parameters for Ti-6Al-4V.

A (MPa)	B (MPa)	n	m	Melting Temp (K)	Transition Temp (K)
862	331	0.34	0.8	1064	980

4. Results and Discussion

4.1. Global analysis of DED-processed components

Detailed results of the global properties of the DED-processed Ti-6Al-4V tensile specimens were outlined in the previous study by the authors [21]. The overall patterns of anisotropic porosity and mechanical behavior of the specimens observed in the previous study motivated the localized approach taken in this work. By comparing the bulk porosity volume fraction and the ultimate tensile strength of the tensile specimens, relationships between mechanical behavior and porosity were clear in certain orientations of the component than in others. Figure 5 illustrates the dependence of mechanical behavior on bulk porosity in the 800 W processed component in the “A”, “B” and “C” orientations. The ultimate tensile strength (UTS) values are normalized by the maximum UTS value observed in DED-processed Ti-6Al-4V, which is about 1200 MPa [39].

Pores due to lack of fusion are results of the large thermal gradients at layer interfaces do not properly fuse together properly. Toward the side surface of the component, there is more spherical and micro-scale porosity due to vaporization, leading to overall more bulk volume porosity closer to the side surface. Close to the top surface, phase transformations occurred over a relatively short time, leading to fast cooling and porosity from shrinkage. Tensile specimens from layers closer to the core of the component had slower cooling and less shrinkage due to re-melting and re-heating from layers above. However, specimens closer to the core of the component also exhibited more vaporization porosity.

Tensile specimens in the “A” orientation, which had its principal load axis in the build direction, exhibited the greatest anisotropy of ultimate tensile strength, as seen in Fig. 5. Mechanical behavior in the “A” direction was highly dependent on porosity in the tensile specimens because of the alignment, shape and size of the pores in the direction. The pores were at the layer interfaces with a spacing of 0.95 mm and aligned throughout the tensile specimens so that about ten rows in the build direction of large, irregularly shaped pores coalesced and led to failure. Not only did the “A” direction tensile specimens had porosity aligned at the layer interface, but also exhibited large thermal gradients throughout the part as the specimens included material close to the bottom of the part as well as the top, or about ten layers in the build direction.

Tensile specimens in the “B” direction had a principal load direction in the hatch direction. Mechanical behavior in the “B” direction was also dependent on porosity but not to the degree that the tensile specimens in the “A” direction were dependent. The rows of pores in the “B” specimens were aligned at the hatch spacing between each clad of the same layer, which were 1.25 mm apart, resulting in about eight rows in the X axis of large, irregularly shaped pores. Because each tensile specimen only included material from one or two layers in the Z axis with material from about eight hatched clads, the thermal gradients throughout the specimens were not as large as those in the specimens in the “A” direction. Tensile specimens closer to the core of the component had slower cooling and less shrinkage due to re-heating from layers above. However, specimens closer to the core of the component exhibited more vaporization porosity.

Tensile specimens in the “B” direction had a principal load direction in the scan direction. Mechanical behavior in the “C” direction was not as dependent on porosity as the behavior in the “A” and “B” directions. This is because the tensile specimens included material from two or three layers in the Z axis and a single clad, or hatch, in the X axis. Thus, not only was there less thermal gradient in tensile specimens in the “C” direction, but pores were not aligned in rows normal to the load axis of the tensile specimens machined in the “C” direction. Though there was a trend of increasing ultimate tensile strength with proximity to the core of the component due to an increase in martensitic formation and more re-heating at the core, there was no clear trend of increasing bulk volume porosity with proximity due to the changing type of porosity in the “C” orientation from shrinkage at the surface to vaporization closer to the core of the cube.

Figure 5: Relationship between bulk porosity and mechanical behavior in three orientations for 800 W.

In Fig. 5, each data point is labeled by its tensile specimen designator as follows. The letter denotes the orientation and the numerical value denotes how far the specimen was from the surface of the component. Subsequent specimens were 1.5 mm away from the previous specimen that was closer to the surface. For example, the data label “A1” denotes a specimen in the “A” orientation and immediately close to, or 1.5 mm from, the surface, whereas “C7” denotes a specimen in the “C” orientation and the seventh specimen from the surface, or 10.5 mm from the surface of the component. Figure 5 illustrates the importance of the shape, size and dispersion of pores and the direction of tensile load, with specimens

near the surface of the cubic component usually failed at lower elongation.

The dependence of mechanical behavior on the orientation of the tensile specimen within the bulk component is further illustrated in Fig. 6 for those tensile specimens on the surfaces of the cube. Specimens in the “C” orientation exhibited greater ductility and higher load bearing capacity than those in the other orientations. This phenomenon is **because** specimens in the “C” orientation did not experience changes in the hatch direction nor in the build direction, and hence, less porosity due to lack of fusion at the layer or hatch interfaces throughout the principal load axis as those specimens at the “A” and “B” orientations would. The results shown in Figs.5 and 6 illustrate the need for a deeper understanding of orientation- and location-dependent behavior, such as shearing or crack initiation, which is dictated by the thermal history of localized areas.

Figure 6: Stress-strain curves of tensile specimens in three orientations in the 800 W component.

4.2. Localized analysis

The localized analysis combined numerical results from a thermal model with experimental 2D micrographs to illustrate porosity distribution throughout the component. The results established relationships between cooling rate, microstructure and mechanical behavior in the **proposed framework**.

4.2.1. Solidification cooling rate

The output of the thermal model was the thermal history at every node during the DED build. A snapshot of the build at about 5000 seconds showed that the melt pool was near the front of the component as a new layer fused with the subsequent layer as shown in Fig. 7. The melt pool was represented by red elements that had temperatures greater than the melting temperature, i.e., greater than 1877 K. The group of red elements that represented the melt pool totaled to about 15 mm³ at any given time throughout the build. Compared to the melt pool volume throughout the build, the element size of less than 0.4 mm³ was refined enough to resolve the thermal gradient within the melt pool. The model captured the rapid cooling of the component while subsequent layers underwent re-melting cycles when the laser traversed over. Figure 7 shows the 800 W processed component at a point and time window while the model's outputs for the 710 W and 940 W processed components (not shown here) showed similar re-melting cycles and melt pool evolution at the same point and time window but slightly different numerical values.

Figure 7: Melt pool evolution during the model's element birth; thermal history of a probed point (highlighted green element) with the solidification rate calculated at the circled re-melting cycle.

The thermal history at any point of the component can be plotted to show the solidification cooling rate between the liquidus and solidus temperatures at multiple re-melting cycles, as denoted by the dotted lines in Fig. 7. 2D porosity micrographs were taken at the probed points of the thermal model. The solidification cooling rate values at these points completed the first link in the framework and were shown to have relationships with porous microstructure at the same points.

4.2.2. Dependence of pore descriptors on solidification cooling rate

2D binary micrographs were taken at localized areas aligned with the probed points with calculated solidification cooling rates from the thermal model, as shown in Fig. 8. The size, shape and distribution of the individual, aligned interlayer pores in the cubic component led to proper characterization of the relationship between the DED process parameters and mechanical behavior. Each pore was assumed to be an ellipsoid and had semi-principal axes lengths of a , b , and c , per the XYZ coordinate system. The dimensions of the pores changed

with direction and location within the cubic component. Due to more frequent re-melting, porosity at bottom layers tend to be more irregularly shaped and less common than those in top layers and locations closer to the surface of the component. As seen in Fig. 8, many areas of the component exhibited aligned porosity with layer thickness spacing, hatch spacing, or both. Pores in Fig. 8 also ranged from irregularly shaped on the left side toward more spherical pores. Though the cubic component had a relatively simple geometry, the heat transfer and resulting solidification cooling behavior at every point in the build was highly variable and complex, particularly at the start and end points of the tool path within a layer.

DED processing of more complex geometries require an understanding of the microstructure and solidification cooling behavior at every area to guarantee structural integrity. Localized study on cubic components is a step into gaining insight into how porosity microstructure and solidification cooling are linked.

Figure 8: 2D porosity map at the same point the solidification cooling rate was calculated in Fig. 7.

By linking the predicted cooling rate, pore shape and dispersion descriptors, a gradient of interlayer and intralayer porosity appeared as solidification cooling rate increased. Larger, irregularly shaped interlayer pores appeared when the solidification cooling rate increased due to lack of fusion and thermally-driven volume change at the melt pool. On the other hand, there were fewer interlayer pores, leading to a decreased area fraction of pores and increased nearest neighbor distance as solidification cooling rate increased. These relationships are illustrated in Fig. 9.

The fit types for Fig. 9 were selected because they fit well with the experimental data, with the fits tested by calculating residuals and goodness of fit tests like RSME. The fit types were reasonable with the experimental data because of the relationship between increasing solidification rate and the exponential decay of solute, or pore concentration relative to the distance from the solid-liquid interface during solidification [40, 41]. The shape descriptors of the pores, including the number of pores and pore shape, are related to the spatial and temporal concentration of pore concentration and behavior that changes with solidification cooling [40, 41, 42].

Figure 9: Relationship between simulation-determined solidification cooling rate and experimentally-determined (a) pore size, b) pore roundness, c) area fraction of porosity and d) dispersion of pores measured using average nearest neighbor distance (NND).

Figure 9a plots the *average pore size* at each point where the solidification cooling rate of the last re-melting cycle was probed. As the solidification cooling rate increased, the average pore size also increased most probably due to the presence of more irregularly shaped, lack of fusion pores. In addition, the standard deviation of the pore size also increased with increasing solidification cooling rate, as the heterogeneity of the porosity microstructure increased. The relationship between the experimentally-determined average pore size and computationally-determined solidification cooling rate was found to have a logistic growth function, defined by a shape descriptor, S_{size} in the following equation:

$$S_{size} = \frac{A_{size}}{1 + B_{size} \exp(-C_{size} \frac{dT_{liq \rightarrow sol}}{dt_{liq \rightarrow sol}})} \quad (7)$$

where $\frac{dT_{liq \rightarrow sol}}{dt_{liq \rightarrow sol}}$ is the calculated solidification cooling rate between the liquidus and solidus

temperatures. Parameters for the logistic growth function are given in Table 5.

Table 5: Pore size parameters for logistic curve-fit.

Pore size parameter	Value
A_{size}	$7.00 \times 10^3 \mu m^2$
B_{size}	1.40×10^2
C_{size}	3.65×10^{-3}

The logistic growth function is a statistical model that predicts a period of growth as a descriptor value transitions from exponential growth to slow growth once a saturation limit is reached. Physical limits in the DED process, in particular the solidification velocity due to diffusion of solute in the liquid Ti-6Al-4V, slows the growth of the pore size descriptor and dominates the saturation limit [43]. The logistic growth function has been used in solidification modeling, including those that incorporate neural networks [44] and smooth modeling based on the latent heat evolution approach to evaluate the volume liquid fraction function during solidification [45].

Figure 9b plots the *average pore roundness* at each evaluated solidification cooling rate. As the solidification cooling rate increased, the average pore roundness decreased because of the increased of irregularly shaped pores. The relationship between the experimentally-determined average pore roundness and computationally-determined solidification cooling rate was an exponential decay function. Exponential decay relationships are observed in heat transfer applications and in the concentration of liquid media in binary and ternary alloys during solidification [46]. The exponential decay function for pore roundness during solidification is defined by a shape descriptor, S_{round} in the following equation with parameters in Table 6:

$$S_{round} = A_{round} \exp(-B_{round} \frac{dT_{liq \rightarrow sol}}{dt_{liq \rightarrow sol}}) \quad (8)$$

Table 6: Pore roundness parameters for exponential decay curve fit.

Pore roundness parameter	Value
A_{round}	1.6
B_{round}	1.2×10^{-3}

Figure 9c plots the *porosity area fraction* at each evaluated solidification cooling rate. As the solidification cooling rate increased, the **number of pores** decreased due to sufficient melting and fusion of the titanium alloy powders. The relationship between the experimentally-determined porosity area fraction and computationally-determined solidification cooling rate was an exponential decay function. The curve fit suggests that the porosity in the Ti-6Al-4V component built with the given process parameters did not achieve less than a 0.2% area fraction. Hot isostatic pressing (HIP'ing) is required for a denser part, though an optimized

combination of process parameters may achieve full density. A previous study on porosity in cast aluminum alloy [47] suggested that gas diffused porosity follows an exponential decay function because with increasing cooling rate, the less time entrapped gas can diffuse into pores. The exponential decay function for porosity area fraction during solidification is defined by a shape descriptor, S_{frac} in the following equation with parameters in Table 7:

$$S_{frac} = A_{frac} \exp(-B_{frac} \frac{dT_{liq \rightarrow sol}}{dt_{liq \rightarrow sol}}) + C_{frac} \quad (9)$$

Table 7: Porosity area fraction parameters for exponential decay curve fit.

Porosity area fraction parameter	Value
A_{frac}	8.416×10^{-2}
B_{frac}	1.261×10^{-3}
C_{frac}	2.000×10^{-3}

Figure 9d plots *porosity dispersion* in terms of nearest neighbor distance for every pore at each evaluated solidification cooling rate. As the solidification cooling rate increased, the distance between each pore increased due to the number of pores decreasing. This suggests that less **less spherical pores due to entrapped gas and more irregularly shaped pores due to lack of fusion occurred at greater cooling rates**. Gas entrapped pores were not restricted to aligned spacing of layer thickness or hatch spacing, and therefore, were found to be closer to other pores. The relationship between the experimentally-determined porosity dispersion and computationally-determined solidification cooling rate was a logistic growth function. This function is related to the pore size, roundness and area fraction, as the distance between each pore depends on these shape descriptors. The physical limits that determines the saturation value are the process parameters, most notably the layer thickness and hatch spacing where more pores due to lack of fusion occur. The logistic growth function for porosity dispersion during solidification is defined by a shape descriptor, S_{disp} in the following equation with parameters in Table 8:

$$S_{disp} = \frac{A_{disp}}{1 + B_{disp} \exp(-C_{disp} \frac{dT_{liq \rightarrow sol}}{dt_{liq \rightarrow sol}})} + D_{disp} \quad (10)$$

Table 8: Pore dispersion parameters for logistic curve fit.

Pore dispersion parameter	Value
A_{disp}	$6.566 \times 10^2 \mu m$
B_{disp}	1.835×10^4
C_{disp}	1.100×10^{-2}
D_{disp}	$1.484 \times 10^2 \mu m$

Localized analysis of the porosity descriptor dependence on solidification cooling completed the second link in the **framework** to connect cooling rate and porosity. Relationships between porosity descriptors and process parameters controlled characteristics, such as solidification cooling rates, are applicable for prediction purposes. **The** ability to probe the cooling rate of DED-processed components with complex geometries would aid the prediction of types of porosity and its descriptors in specific locations of the component. Furthermore, knowledge of porosity and its descriptors can provide statistically representative elements to predict mechanical behavior at localized areas.

Limitations to the analysis that evaluated the relationships between porosity descriptors and solidification cooling are that there exist nuances in both experimentally and computationally determined data. Porosity presented in 2D micrographs may not be fully representative of the localized microstructure of the part due to differences in the machine environment during a build. The thermal model presented in this study was not calibrated or validated yet and only served as a qualitative means of comparison. Other physical phenomena such as volume change of elements was not captured in the thermal model. The presence of alpha, beta and martensitic phases in the microstructure can provide more information on phase changes and resulting mechanical behavior. **However, identifying relationships between cooling and microstructure provide a valuable step in the overall proposed framework. This is particularly vital with DED-processed components with complex geometries and varying thermal histories and structure.**

4.2.3. Statistically representative porosity maps and mechanical behavior

The last link in the **three-link chain framework** connected the porosity size, shape and dispersion to mechanical behavior. Using the relationships between cooling rate and porosity established in the previous section, statistically representative porosity maps can be generated and incorporated into representative volume elements. Figure 10 is an example of a meshed 2D representative map at a solidification cooling rate of 750 K/s. The 2D finite element geometry was composed of two materials air in the white void areas and Ti-6Al-4V as the matrix, defined by the Johnson-Cook damage model.

Figure 10: Statistically representative porosity map and its resulting FEA mesh.

By modeling the 2D representative element as a uniaxial tensile test specimen, shear bands and void coalescence were present and were assumed to lead to failure. Other than using the Johnson-Cook hardening law of the matrix material, Ti-6Al-4V, there were no damage or failure models embedded in the RVE, therefore, there was no softening behavior

currently predicted from FEA. Nevertheless, the incorporation of the damage model in the matrix material can be incorporated in future work. The mechanical behavior of a sample consisting of a porosity map corresponding to a solidification cooling rate of 750 K/s was comparable to global mechanical properties in Fig. 6 of the tensile specimens, as shown in Figs. 11a-d.

Figure 11: Shear bands and stress fields surrounding pores for a cooling rate of 750 K/s with the resulting stress-strain curves for the localized are: (a) the load is applied at the right of the RVE; (b) the load is applied at the top of the RVE; (c) the load is applied at a 45 angle; (d) All three local RVE curves with the global stress strain curves (see Fig. 6) at the three tested orientations.

Figures 11a-c show the RVE with applied load at three different orientations and show how the localized pores change shape depending on the alignment and orientation. Figure 11d shows all three localized ABAQUS results with the global experimental results. Compared to the global experimental results in Fig. 6, the local mechanical behavior also exists as variation in the elastic modulus with orientation, and the modulus is highest for the “C” direction because of the lack of aligned pores in the tensile specimens in that direction.

Hence, mechanical behavior can be observed on a point-by-point basis and the **proposed framework can ultimately predict properties** at localized areas.

5. Conclusions

DED-processed components exhibit highly inhomogeneous and anisotropic behavior due to the distinguished thermal histories in each localized area, which are highly dependent on process parameters, tool path, component geometry and material compositions. Porosity is a microstructural feature found in many DED-processed components. Larger, irregular shaped pores were more prevalent in areas with greater solidification cooling rate due to lack of fusion, whereas areas with lower solidification cooling rate resulted in vaporization and gas entrapped pores.

This study implemented a **framework** approach to investigate the relationships between the process parameters as inputs into melt pool evolution, the cooling rate during solidification of the melt pool, the porosity patterns and the resulting mechanical behavior at the melt pool. Localized information within AM materials is required to predict for potential points of failure and for process control. The size, roundness and dispersion of pores provides sufficient information for modeling for various types of damage. The statistical relationships between experimentally-determined porosity descriptors and simulation-determined solidification cooling rate in this study can lead to reduced order modeling efforts. Ultimately, these efforts enable the prediction of structure and behavior as a function of process parameters and closed-loop “online” monitoring during the DED process. Monitoring of the process leads to desirable parts and increased confidence in AM, which can fuel large-scale production of high-functioning parts and new materials. Furthermore, “online” monitoring for denser parts avoids additional cost and time for post-processing, such as HIP’ing. A better understanding of local relationships and properties furthers AM research and heightens the capabilities of AM materials.

Ongoing and future work include validating and calibrating the in-house thermal model by using a global IR camera for the component and a point-based IR pyrometer for melt pool sensing. Improved imaging and control techniques can allow for control of the solidification cooling rate as well as uniform material properties. Methods of porosity detection and classification are underway, including X-ray micro-tomography experiments and investigating porosity due to lack of fusion separately from porosity due to vaporization and whether the melt pool exceeds boiling point of the material. Refined finite element analysis of the porous representative volume elements will implement 3D porosity maps and better meshing methods for hexahedral elements. Multi-scale porosity assessment will be implemented into a modified GursonTvergaardNeedleman material model to predict ductile behavior of a variety of DED-processed materials.

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