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REVIEW OF AM SIMULATION VALIDATION TECHNIQUES

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Abstract

Due to the complexity of Additive Manufacturing (AM), it can require many trial runs to obtain processing parameters which produce a quality build. Because of this trial and error process, the drive for simulations of AM has grown significantly. Simulations only become useful to researchers if it can be shown that they are true representations of the physical process being simulated. All simulations have different methods of validation to show that they are an accurate representations of the process. This paper explores the various methodologies for validation of laser based metal AM simulations, focusing mainly on the modeling of the thermal processes and other characteristics derived from thermal history. It will identify and explain the various validation techniques, specifically looking at the frequency of reported use of each technique.

Introduction

Additive Manufacturing is a complex and generally uncharacterized field of study and many have attempted to generalize the process using mathematical models. In order to show the validity of each model, researchers have developed methods to compare the results from these simulations to experiments which can be performed. Each aspect of the AM process which is being simulated will have a different technique for validation. The main phenomena of AM which have been studied are heat transfer, induced stress, and microstructure. For each of these phenomena, the various validation techniques which have been used in literature will be investigated including a brief description of the technique fundamentals.

Heat Transfer Validation Techniques

The most fundamental, and first developed, process in AM which has been modeled is the flow of heat through the part. This problem was first tackled by those interested in simulating the welding process and much can be derived from their work. A very extensive review, [1], has been performed from which key elements can be utilized. The first numerical solutions which can be applied to the problem of AM, [2], created a 3-D finite difference model to simulate a Gaussian laser on a semi-infinite work piece. Their model did not include temperature dependent material properties, which was later remedied [3]. This later iteration also accounted for latent heat of phase change which has been recently realized as an important aspect of AM simulations. The

last simulations developed, which is the most applicable to AM, is multi-pass welding [4, 5, 6]. In these models the laser is passed over the same area multiple time to determine the heat flow due to the multiple passes. These simulations were the first time that "quiet" elements were utilized. These elements are considered inactive until the part has been built up to their location. At this time they are activated and are included in the simulation. This model has been the foundation that most AM simulations have been built upon.

In order to validate these models, thus far in literature, there have been two approaches. The first is to validate the thermal model with an instrument equipped to measure temperature. If this has not been done, then the researchers will measure another physical characteristic of the build and use that to show the model's validity. A representative set of papers have been presented in Table 1. These papers show that a few more attempts have been made to validate using instru-

Table 1: Breakdown of Validation Techniques

Instrument Validated		Physical Char. Validated	
IR/CCD Camera	[7, 8, 9, 10]	Melt Pool Depth	[11, 12, 13]
Pyrometer	[14, 15]		
Thermal Couple	[16, 15]		

mental validation as opposed to using another physical characteristic. This is most likely due to the direct link between the measured value and the simulated value. When using another physical characteristic, it is necessary to know the exact linkage between the trait being measured and the one being simulated. For this reason, there are more opportunities for error and false validation, or rejection, of a given model. From the literature reviewed, there are three prominent instruments which have been used to validate the models.

The most common of these is to use an IR or CCD camera, these cameras are appealing based on several features. The first is that this is a non-contact measurment. Additionally, they are capable of capturing data at a high frame rate, [7] reports frame rates as high as 800 frames/sec. In addition to the high frame rate, these cameras can have a moderate resolution, [8] reports a camera of 256 x 256 pixels where each pixel is 0.1 x 0.1 mm. These capabilities allow researchers to quickly and accurately assess the surface temperature of a build. This method of measuring temperature is not without its faults. The first is that these cameras are very sensitive to the angle and distance they are placed from the object begin measured [17]. Additionally, these cameras measure a time averaged temperature of the skin of the object being heated. This problem does not apply to CW lasers, however, when using a pulsed laser the skin temperature can spike very rapidly which can result in inaccurate measurements [18].

The next instrument most commonly used is a pyrometer, which is a non-contact spot measurement. This results in the ability to measure the average temperature of a specific area. This is not as useful as cameras previously presented due to the lack of resolution. Because of their simplicity, however, it is possible to create a mathematical model to predict the pyrometer results. This has allowed for some to create a model which includes a pyrometer to control the laser power. This simulation is able to predict the changes that the pyrometer will make to the laser power in order to keep a constant melt pool size [14].

The last method found in literature to measure the temperature directly utilizes thermocouples, which are contact spot measurements. The fact that they must be fixed, welded in most cases, to the

surface makes them impractical for some applications, such as powder bed temperature validation. In addition, they will only record the temperature average of a specific location. Therefore, in order to obtain an accurate representation of the temperature profile, several thermocouples need to be placed along the working surface. Another large downfall with thermocouples is their inability to measure the melt pool temperature. Since they need to be fixed to the surface, if an attempt is made to measure the melt pool they will become detached from the substrate and the data will be invalid. For all of these reasons, current researchers have only used thermocouples as a secondary validation technique and utilize another technique for the main source of data.

Besides these direct methods of validating the thermal modeling, some researchers have taken the approach of measuring a more easily attained data set and comparing that to the simulation, namely the melt pool size and the shape of the build. In this method a simple surface laser heating

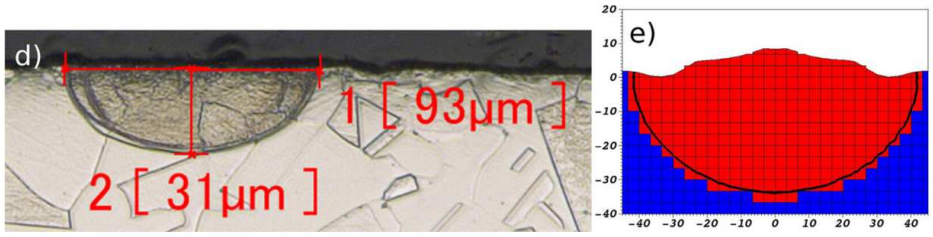

Figure 1: Validation of thermal analysis by comparing melt pool dimensions of experiment (left) and simulation (right) [12]

simulation and experiment are performed, where the laser is simply used to melt a tract on the surface of the substrate. In the experiment a slice is taken perpendicular to the laser path which is then analyzed, typically with an optical microscope. This allows for the width and depth of the melted region to be measured, as seen on the left image in Figure 2. In the simulation, since the temperature is tracked for each element, it is possible to flag elements which have melted, this is done in the right image in Figure 2 by changing their color to red. In addition to the use of the surface laser heating, some have simulated a single track build.

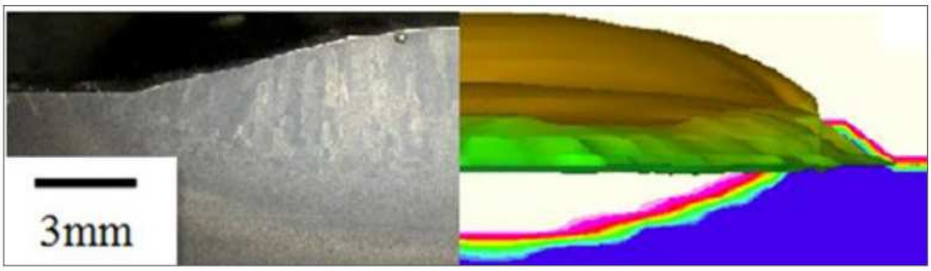

Figure 2: Validation of thermal analysis by comparing single track build dimensions of experiment (left) and simulation (right) [13]

This indirect method of validation can typically be done without specialty equipment. However, this method of validation introduces new complications which can hide, or skew, the results. Since the material is melted, the flow of the molten material dictates the shape of the melt pool. For that reason, this validation technique requires that both the thermal model and the fluid models are correct. Therefore, the direct methods are simpler to implement than the indirect methods.

Stress Validation Techniques

Throughout the AM process, the cyclic heating which is applied to the part leads to stresses being induced. The stressing process has been divided into four stages. Stage A occurs when the heat source approaches a specific location on the part. This stress is compressive since the volume under the heat source is expanding. This compressive stress is elastically compensated for by the material until the compressive yield stress limit is surpassed. When the compressive yield limit is surpassed, stage B takes place. In this stage plastic flow of material occurs, and the compressive stress is reduced. Stage C has begun when the material begins to cool which results in tensile stress. These stress are induced by the contraction of the material begin restrained by the surrounding material. These stresses remain elastic until the tensile yield stress is surpassed. The final stage of stress is stage D, which occurs when the tensile yield limit is surpassed and plastic flow begins [19]. These stresses can all be derived from the thermal history of a specific location and its neighbors. Due to the difficulty of measuring the stress, only a few methods have been used throughout literature which are displayed in Table 2.

Table 2: Frequency of Stress Analysis Techniques

Presence of Cracks	[9]
Neutron Diffraction	[19, 20]
X-Ray Diffraction	[21, 22]

One of the simplest, though not an extremely accurate method, is to observe the creation of cracks within the part and compare that to simulation results. This method is very simple and can be done with without any specialty equipment. This method however, due to its lack of precision can only be used to qualitatively verify that a simulation is giving results which generally agree with the experiment. This method can not be used to quantitatively validate a mathematical model [9].

In order to quantitatively validate the simulation, the exact stress, or strain, values need to be known from experimental work. This is done using Bragg's Law and the scattering of either X-Ray's or neutrons. To obtain the spacing, the part is placed in the apparatus and the diffraction patterns are recorded from various angles. This allows for a baseline pattern set which gives the current spacing for all the atoms. The part is then put through the thermal process being investigated which will move the atoms. This motion will induce a stress based on the amount the atoms have been moved. The difference in the diffraction patterns directly correlates to the distance that the atoms shifted. This motion of atoms is known as the strain which can then be converted to stress using Hooke's Law [23].

This method of determining the stress locally allows for a direct correlation between the experiment and simulation. The choice of neutron or X-Ray is based mainly on availability to the researchers. The use of X-Ray Diffraction (XRD) is much more widely available to researchers and therefore a more cost effective method, whereas the use of neutrons is only done in specific facilities. One of the downfalls of these strain measurments is their inability to be used in-situ, therefore the measurments can not be used throughout the AM process and only the final results can be compared. In addition to the localized strain, some have used distortion measurements from 3-D scanners to further verify the simulations results [20].

Microstructure Validation Techniques

Due to it's many desirable characteristics, namely its high strength to weight ratio and corrosion resistance, Ti-6AL-4V (Ti-64) will be the focus of this section. In order to obtain the optimal strength the microstructure of the build is critical. Because of this, many researchers have developed models to determine the microstructure of an AM build.

To understand the modeling of the microstructure of Ti-64 it is necessary to study the microstructures that can occur. Ti-64 has a microstructure which is a combination of a body centered cubic (BCC), which is denoted as a β phase, and a hexagonally closed packet (HCP), which is denoted as an α phase. These phases will coexist within the Ti-64 part and the quantities and sizes will depend on the maximum temperature and cooling rate at a specific location. At room temperature the typical microstucture is $\alpha + \beta$. If the materials temperature is raised higher than the beta transus temperature the material will transition into pure beta phase. As the material cools, the alpha phase will reappear and the cooling rate will dictate which alpha phases occurs. This is shown

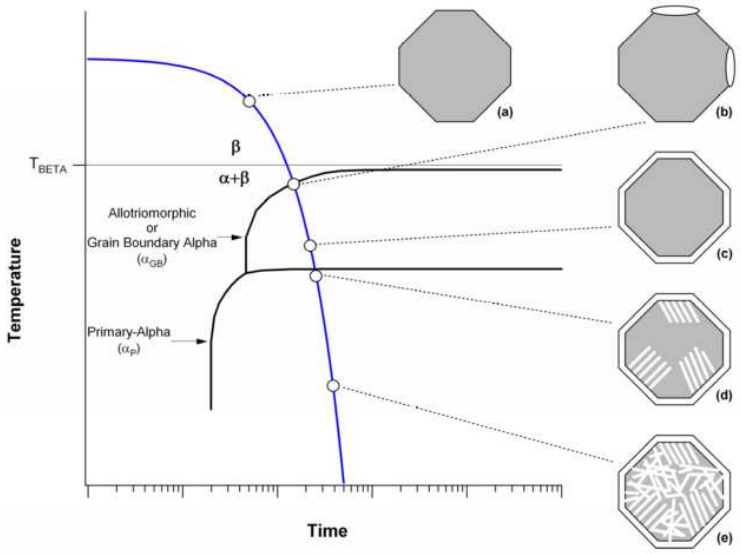

Figure 3: Illustration of phase transformations which occur in Ti-64 [24]

graphically in Figure 3. If the cooling rate is fast then the resulting alpha phase will be Martensitic (α') or Massive (α_m). These phases will appear intragranularly and on the grain boundaries respectively. On the contrary, if the cooling rate is slow then the resulting microstucture will start with Allotriomorphic (α_{GB}) on the grain boundaries followed by primary-alpha (α_P), which is simply any alpha phase that appears from cooling above the beta transus temperature, which is shown in the back-scattered electron (BSE) graph in Figure 4. Lastly, when the material containing $\alpha_P + \beta$ is heated, but not past the beta transus temperature, some of the α_P will convert to β. When this material then cools, the new phase created is called secondary-alpha (α_S). This secondary phase becomes critical in AM due to the constant reheating from the layer by layer manufacturing strategy [24]. Based on this understanding of the microstrucutre evolution there are a few methods of quantifying, and therefore validating, a simulation.

In the first simulation method the models elements are only allowed to be one of the various phases. Based on the elements thermal history it is denoted as either beta or one of the alpha

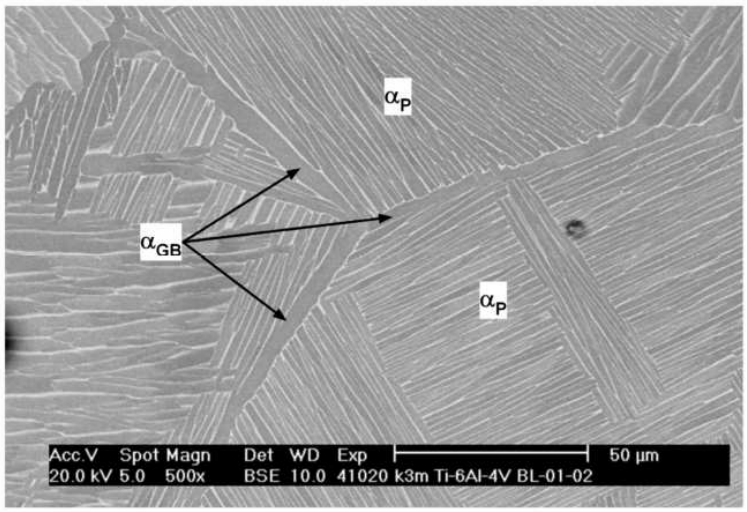

Figure 4: Illustration of phases of Ti-64 [24]

phases. This allows for a very general comparison with experimental results. When a thin wall is built, it can be sliced perpendicular to the laser scanning direction. This slice can then be observed with the scanning electron microscope (SEM). These images will then produce distinct regions, as shown in Figure 5, of each phase which can be compared to simulations [25].

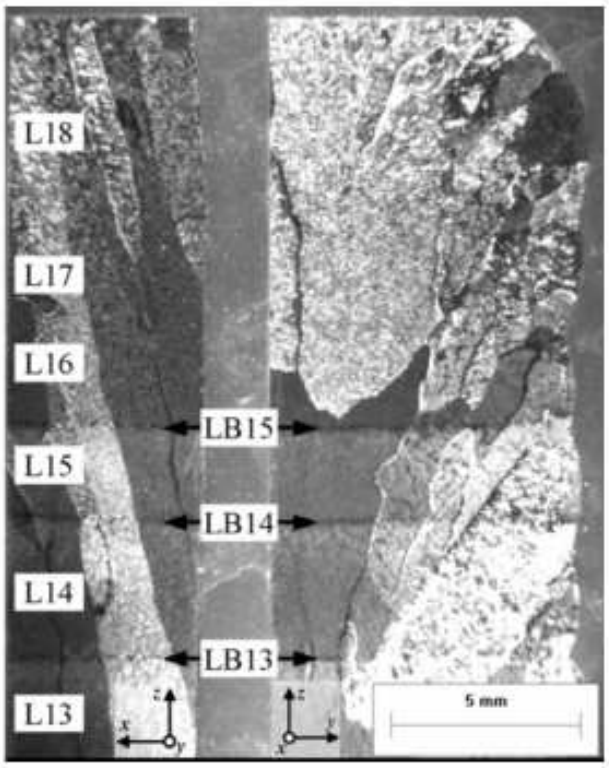

Figure 5: Phase layers of Ti-64 produced via thin wall deposition [25]

This simplified method is a fundamental start but is very lacking. It is known that the grain

size, morphology, and distribution of fine particles is just as important to the mechanical properties and the phase itself. Therefore, researchers have attempted to model the grain size along with the phase. The simplest of these validations uses the volume percent of each of the phases. To ensure that the model is correct, several cooling rates were modeled and compared to experimental results. When several cooling rates simulated matched experimental results, the simulation was considered correct, which is illustrated in Figure 6 [26]. Another method of validating the microstructure is

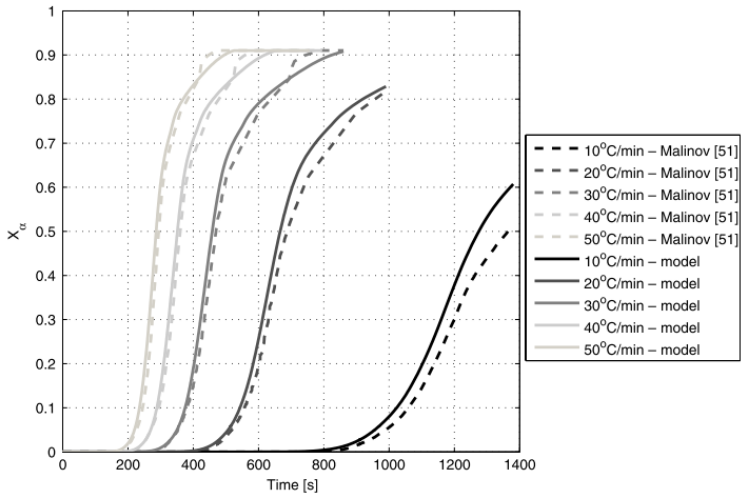

Figure 6: Volume fraction of alpha phase comparison [26]

by comparing the size distribution of the alpha phase. To compare the size distribution of the alpha phase, the average width of the alpha phases can be calculated and this can be used to compare the simulation to the experimental data [27]. In order to be more rigorous, a histogram of the sizes of the alpha phase sizes and the volume percent of the phases can be utilized [28]. All in all, if a more detailed and rigorous a validation technique is used the simulation can be more trusted.

Conclusion

This paper presents the main validation techniques in literature for the validation of thermal modeling of AM and other attributes which are related to the thermal history. The heat transfer in the build can be measured using either direct or indirect means. The direct means include the use of cameras, pyrometers, and thermocouples. These methods give a direct link between the mathematical models and the experimental data. The indirect methods of validation use the melt pool dimensions to show that the simulation is correct. This method relies heavily on the fluid model being correct as well as the correctness of the thermal model. Because of this, it can be preferred to use a direct method of measuring the heat flow.

Closely linked to the thermal history are the stresses induced in the build. In order to verify a simulation, some have used the presence of cracks. This is only a rough correlation and in order to be more precise diffraction needs to be utilized. This measures the strain in the material which is directly linked to the stress.

In addition to the stress, the microstrusture of Ti-64 is mainly dependent on the thermal history. The validation of this simulation can take to crude form of validating based solely on the phase

present. A more rigorous approach involves with calculating the percent volume of each of the phases and comparing these values. In addition, the size distribution of a phase can be found which can be used for further validation. All in all, the validation of a simulation is very critical and sometimes overlooked step. The selection of a validation technique must be appropriate for the simulation which is being created.

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