Predicting the Properties of Additively Manufactured Parts

Tyler London¹, Damaso De Bono¹, Victor Oancea² and Sakya Tripathy²

¹TWI Ltd. ²Dassault Systèmes SIMULIA

Abstract: Selective laser melting (SLM) is an additive manufacturing (AM) process whereby a laser produces a three-dimensional part by selectively fusing regions of a metal powder bed in a layer-wise manner. SLM has the ability to produce complex, light-weight, metallic parts with the potential to reduce costs and lead times over conventional manufacturing processes. However, the layer-by-layer nature of the SLM process introduces an almost unique thermal history at each location within the part as subsequent laser passes reheat the material. As a consequence, strong microstructural anisotropy and hence location-dependent material properties are features of SLM builds. The ability to accurately simulate and predict the distortion, residual stress and microstructural evolution that arise from this process is therefore crucial to establish SLM as a robust and reliable manufacturing route.

In this paper, thermo-mechanical-metallurgical simulations of Ti-6Al-4V parts produced by SLM are validated against experimental measurements. The work involves the simulation of the SLM process and the prediction of location-specific microstructural features (such as grain size, morphology characteristics and phase fractions). A framework for more generally predicting the mechanical properties of printed parts is then presented. This involves the implementation of a novel mapping between microstructural quantities and tensile properties at each material point. The results demonstrate the potential that the powerful new features of Abaqus2017 have for simulating AM processes.

Keywords: Selective Laser Melting, Additive Manufacturing, thermo-mechanical simulation, metallurgical predictions, Ti-6Al-4V.

1. Introduction

Selective laser melting enables the production of near-net-shape components layer-by-layer using 3D computer aided design (CAD) data. This process has the potential to significantly reduce material wastage, energy usage and component lead times whilst enabling light-weight designs to be built that could not otherwise be made with conventional casting or subtractive manufacturing technologies.

Ti-6Al-4V (Ti64) is one of the most widely used α+β dual-phase titanium alloys and has been adopted as one of the key powder metallurgies for additive manufacturing. Due to its broad applications in biomedical devices, aerospace, marine and offshore applications, Ti-6Al-4V parts fabricated by SLM have been investigated extensively (Zhao et al, 2016). Whilst there is
significant microstructural anisotropy in AM components, there has been little effort in the past to understand the connection between the anisotropic microstructure and the macroscopic mechanical properties (Carroll et al, 2015).

The objective of this study is therefore to demonstrate that:
1. the metallurgical characteristics of Ti-6Al-4V parts processed by selective laser melting can be predicted using new features of Abaqus, and
2. the proposed methodology can then be extended via a phenomenological approach to map location-specific mechanical properties onto the part, thereby enabling predictions of the strength of the anisotropic SLM part.
3. The approach taken involves a thorough experimental test programme and detailed numerical modelling of the AM processing. The measurements made on the SLM test pieces are then compared with the finite element predictions. The next steps required to advance the current work programme are then discussed.

2. Experimental Approach

2.1 Geometry and SLM Build Parameters

The geometry of the SLM build comprised 12 square-section beams on a 16.6mm Ti64 substrate. Three sets of 4 nominally identical beams with a square cross section were built. Beam type B1 had dimensions 2.5 x 2.5 x 20mm; Beam type B2 had dimensions 10.0 x 10.0 x 20mm, and Beam type B3 had dimensions 10 x 10 x 10mm. To produce the beams, TWI Ltd used a Renishaw AM250 with a 250 x 250 x 300mm build volume and a 200W SPI Ytterbium fibre laser. The build chamber is purged with argon gas prior to processing, and the gas is recirculated during the build via a dedicated filter.

All specimens were built with Ti-6Al-4V Grade-23 metal powder supplied by TLS Technik and with a powder particle size range between 15 and 45μm. The substrate was heated to 150°C and the scanning strategy as described below was followed so that the manufacture of the beams would result in >99% density (ie low porosity) in the parts.

The scanning strategy employed conventional 0°/90° alternating layers with the inner region of the part filled with parallel hatch lines, followed by four contours for the boundary. For the hatch lines, the spacing was 80μm with a spot distance of 50μm and a laser power of 170W with an exposure time of 60μs. For the boundary, four concentric contours were traversed with the outermost contour on the boundary and each additional contour separated by 40μm. The spot distance for the contours was 20μm with a laser power of 120W and an exposure time of 60μs. A layer thickness of 60μm was employed. The scanning strategy is illustrated in Figure 1:
Figure 1 Scanning strategy for the SLM beams showing alternating layers.

The beams in the as-built condition prior to removal from the substrate are shown in Figure 2.

Figure 2 Ti-6Al-4V beam samples as-built prior to removal from the substrate.

2.2 Post-processing and heat treatment

Because SLM generates rapid cooling rates, the microstructure in the as-built conditions tends to be predominantly martensitic $\alpha$-phase (or $\alpha'$). Therefore, to provide a more varied microstructure, half of the beams were heat treated. A heat treatment involving a 2 hour soak at 750°C was employed.
2.3 Metallographic examination

Following heat treatment, the beams were cut in half longitudinally. All metallographic samples were cut with an abrasive wheel, mechanically ground and polished and etched with Kroll’s reagent. Size, appearance, density and porosity of each sample were characterised. The microstructure and sample composition were determined using scanning electron microscope (SEM), whilst electron backscatter diffraction (EBSD) and optical microscopy were used to quantitatively examine the phase fractions present at various locations. Figure 4 shows images of the characteristic microstructure from the as-built condition. This shows high concentration of α and α’ martensite due to the rapid cooling arising from the thin structure of the build.

All locations examined in the build show a very fine Widmanstätten type microstructure containing a mixture of the acicular α and the martensitic α’ phases. This structure is characteristic of a fast transformation from the β phase field to the α + β phase field during cooling. Due to the very similar crystal structures it is not possible to reliably distinguish between α and α’ phases using EBSD and therefore both are indexed as α phase; however, the BCC β phase can be readily identified. In the as-built condition no significant quantity of β phase was detected although, it should be noted that the maps shown are not 100% indexed meaning very fine regions of β phase may be present in the unindexed regions which appear black on the EBSD maps and are thus hidden from the images.

In the as-built condition a subtle microstructural transition can be identified moving from the bottom to the top of the column. At the bottom of the column Figure 4 shows small regions of more equiaxed α phase dispersed between the fine laths of the Widmanstätten microstructure. Far fewer of these equiaxed regions are observed at the middle and the top of the build where the structure is dominated by finer Widmanstätten laths.
Figure 4 EBSD map and optical micrograph for B1 as-built (non-heat treated) condition.

3. Modelling Approach

3.1 Overview of the computational framework

New physics-based approaches implemented in Abaqus 2017 were used in this study. The key aspects of the new framework include:

- Machine information: the SLM process-specific information such as the laser scan strategy, powder recoating sequence, and layer thickness is pre-processed with no loss of accuracy from the actual data used by the physical machine. This is handled through the generation of “Event Series” which are arrays of time, position and power for the laser heat source and powder wiper.
- A new Intersection Module is used to sweep through the finite element mesh with the tool path and heat source configurations. This allows for an efficient definition of the heat source without need to reference an underlying finite element mesh (and the latter need not conform to the layers).
- Progressive element activation: at any given point during the simulation, any finite element could be completely filled with matter, partially filled, or empty. The software precisely keeps track of this evolution, the mass inventory and distribution.
- Progressive heating computations: at any point in time, heat bursts are computed by taking into account the actual path and power distribution of the heat source. An arbitrary number of heating events (characterized as a sequence of heat fluxes at given locations) are computed for an accurate representation of the heating source in both time and space.
- Progressive cooling via convection and radiation: partial facet areas are computed to allow for a precise assessment of cooling regardless of the finite element discretization.
3.2 Geometry and finite element mesh

The geometry of the parts and assembly as modelled in Abaqus/CAE is shown in Figure 5. The same positioning of the beams on the substrate as in the test piece was employed in the model.

Figure 5 Image of the Assembly in Abaqus/CAE showing the 12 beams on the substrate.

The FE domain was meshed using 8-node linear brick heat transfer elements (DC3D8) for the heat transfer simulation of the SLM process. The physical layer height for this print was 60 µm and the hatch spacing was approximately the same magnitude; therefore, if an accurate assessment of the effect of layer-by-layer thermal transients arising from the specific laser scan vector would be of interest, then a uniform mesh size of about 0.06mm for the beams (or smaller) would be appropriate. Hand calculations show that such a uniform seed size would result in approximately 600,000 elements for beam type B1 and 10,000,000 for beam type B2. Combined with the need to have a fine temporal discretization, the analysis of the full computational domain for this kind of metallurgical analysis is not feasible.

However, preliminary analyses indicated that the beams were thermally isolated from one another within the build volume. As a consequence, only a single beam was analysed at a time and the size of the substrate surrounding and supporting the beam could be significantly reduced. The reduced computational domain, showing approximately 3.25mm of build height for beam type B1 with a 0.06mm mesh within the beam is shown in Figure 6. A biased mesh was employed in the substrate.
3.3 Material properties

Both the substrate and the beam were made of Ti-6Al-4V. Temperature dependent material models for conductivity, specific heat, and density were chosen.

3.4 Loads and boundary conditions

The initial temperature of the substrate was set to 150°C and the beam elements are inactive at the beginning of the analysis. As described in the previous section, the recoater/wiper sequence data is then used to activate progressively the elements according to the actual printing sequence. The temperature of the powder at the time of activation (26°C) is taken into account. The laser motion is then used to model the motion of laser heat source. For every active element, the power of the laser is integrated over all the time and distance it travels in a particular increment and the integrated flux is then applied to the active elements in accordance with the actual printing sequence. For the purposes of this study, a time increment at most 0.0025s was employed.

Convective and radiative heat loss between the solid build and the surrounding environment (both the 21°C argon atmosphere and time-dependent temperature of the surrounding powder bed) was accommodated through a single convective heat loss definition. The value of this coefficient (and its dependence on temperature) was optimised through axisymmetric simulations where the powder was explicitly modelled. The value employed in this simulation was 2.5 W/m²K. This low value takes account of the reduced conductivity of the unfused powder that surrounds the part as it is built. The convection and radiation boundary conditions are only applied on the active free surfaces which evolve as more and more layers get added. This is all performed in a continuous fashion during the time incrementation sequence.
3.5 Prediction of microstructural characteristics

At each time solution increment, a metallurgical model for Ti-6Al-4V was called. This model used the present phase fractions, cooling rate and current temperature in conjunction with the JMA kinetics (for diffusional transformation) and KM equations (for martensitic transformation) to predict the evolution of phase fractions at each material point.

4. Summary of Findings

The thermal transients observed arising from the laser scan strategy for a given layer are shown below in Figure 7.

![Figure 7 Images of the temperature transients arising from the laser scan vector for a single layer. The images start at the top left, move to the right and then from the bottom right to the bottom left.](image)

The predictions from the metallurgical model indicated that, up to mesh discretization, 100% $\alpha$ and $\alpha'$ would be present in the as-built condition. This agrees with the experimental measurements where, for all regions that could be indexed, only $\alpha$ and $\alpha'$ were measured to be present.

5. Future work

The present work has demonstrated the ability to use the new features of Abaqus to accurately simulate additive manufacturing processes, in particular, selective laser melting. The present work has established that the thermal-metallurgical predictions agree with experimental measurements. The planned future activities include:

- Integrating thermocouples in an SLM substrate (and therefore wholly contained within the build chamber) to provide experimental validation of the temperature history predicted by the FE model. This is challenging due to the closed environment under
which SLM processing takes place, but will provide increased confidence in the representations employed for the boundary conditions.

- Develop a phenomenological map from microstructural properties to mechanical properties. Elastic constants have previously been determined from first principles and experimentally for the α, α' and β phases. A linear mixing rule can be used to assign elastic properties to each element based on its phase fraction content. Previous studies have also determined the individual elastic-plastic tensile behaviour of α and β phases from a continuum level. Therefore, a linear mixing rule can also be used to assign inelastic behaviour to each element based on its phase content arising from the SLM process simulation. Finally, the effect of grain size (lathe thickness) on elongation, yield strength and ultimate tensile strength has been empirically measured so that “knock-down” factors can be implemented based on the microstructural characteristics.

- Build cruciform-type geometries within the SLM machine. After the build has completed, remove the cruciform from the substrate and machine tensile specimens from each cruciform. Undertake tensile testing including digital image correlation. Perform the same exercise using simulations: model the SLM processing and predict the thermal-metallurgical content. Use the phenomenological map to assign mechanical properties to each element; in particular, to the elements within the locations where tensile specimens were removed. Simulate the tensile test and compare the results.

This framework will demonstrate the potential for the mechanical properties of AM parts to be predicted from a simulation level. This opens up significant opportunities for design optimisation and process parameter control, whereby target properties can be achieved through tailoring layer-by-layer scan vectors and laser powers.

6. References


7. Acknowledgement

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