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Thermo-fluid-metallurgical modelling of the selective laser melting process chain

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Abstract

The entire process chain of selective laser melting of Ti-6Al-4V is analysed. First, a thermo-fluid dynamical model is used to investigate the temperature profile during the process and estimate the size and shape of the melt pool. The inclusion of the Marangoni effect improves upon previous work by showing the liquid velocity in the melt pool. Next, this information allows us to estimate the morphology of the grains of a part produced by selective laser melting. Finally, a cellular automata is used to model the microstructural evolution during a uniform heat treatment at the beta transus temperature. It is shown that the model shows good agreement with earlier experimental results.

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Keywords: "selective laser melting; thermal modelling; computational fluid dynamics; microstructural modelling; Ti6Al4V"

1. Introduction

Additive manufacturing (AM) is a manufacturing technique, which allows the production of parts with a large degree of geometric freedom. An example of such an AM technique is selective laser melting (SLM). During SLM, the cross section of the desired part is melted into a bed of metal powder. The build plate is then lowered and the process repeats itself until the part is completed [1]. Because of its novelty, there are still some unsolved problems in SLM. The high heat input from the laser leads to a relatively unique temperature profile during production. Measuring the temperature inside of a part is almost impossible, and therefore it is necessary to employ thermal models to gain insight into the temperature evolution during production. This unique temperature profile also results in a microstructure which is different from what can be expected from traditional manufacturing techniques (such as casting or forging). The current study also investigates this grain morphology. Finally, because of the high residual stresses, which result from the thermal cycles involved in SLM, a heat treatment is necessary after production. Since this work aims to model the complete process chain of SLM, a uniform heat treatment and the resulting microstructural change is investigated. A material commonly used in SLM is Ti-6Al-4V (Ti64), due to its mechanical properties and low density [2], which is also the material this paper focusses on. Ti64 has several possible phase transformations, but for this work two are of particular interest: solidification at 1928 K and the transformation of the HCP martensitic α’ phase into BCC β at approximately 1253 K during heat treatment [3].

Numerical modelling of SLM includes a wide range of physics, e.g. heat conduction, radiation, solidification and melting, material transformation (powder to bulk material transition), fluid flow, thermo-capillary surface tensions, etc. Covering all involved physics in one simulation is not practical. Simplified models are usually proposed to remedy this problem, by considering only proper governing physics. Huang et al. [4] made a heat transfer model for the SLM process and identified the main process parameters affecting SLM. Cheng et al. [5] developed a thermo-mechanical model of the SLM process and investigated the effect of the scanning strategies on temperature and residual stresses. Wu et al. [6] included the effect of the volume shrinkage in their thermal model and subsequently investigated the effect of the process parameters on the shape of the melt pool. It is worth mentioning that all the aforementioned papers neglect the fluid flow motion in their models, mainly because of its
relatively high complexity and computational cost. Including the fluid flow motion in laser-based processes, will not only result in a more realistic thermal field [7,8], but will also give valuable information about the solidification process occurred during these processes [7,9].

For microstructural models, this work uses a cellular automata (CA), because it is relatively easy to implement. However, it allows the inclusion of complex physical phenomena. Recently, the CA method has gained a lot of interest. The work of Zinovieva et al. [10] investigated the use of a CA for SLM. Their work is based on the works performed by Rappaz and Gandin [11], who were among the first to model the evolution of microstructure during solidification. Their model allows the CA to become independent of the mesh by using the growth velocity to couple time inside of the model to real time. There are also some studies which model the microstructural evolution of a Ti64 part during heat treatment (most notably the work by Su et al [12]), but these studies are more scarce. In order to find an expression for this growth velocity of grains during heat treatment, empirical relations are used [13].

The first part of this paper develops a macro thermo-fluid numerical model of the SLM process of Ti64 in a Eulerian framework and gives a detailed description about the evolution of the melt pool and liquid flow patterns. Moreover, a metallurgical sub-model is developed and coupled to the mentioned macro model, which gives the solidification parameters like temperature gradient, cooling rate and growth velocity. The results of this sub-model are able to determine the grain morphology, namely whether the grains are columnar or equiaxed. This morphology is then used as an input for the microstructural model, which simulates the final microstructure after a simple heat treatment.

2. Models

2.1 Thermal model

In this paper, a macro thermo-fluid dynamical model has been developed in COMSOL by implementing computational fluid dynamics (CFD). The heat balance equation can be expressed as:

$$\nabla \cdot (\rho C_v \mathbf{u}) + \rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) - \rho \Delta H \left( \frac{\partial f_s}{\partial t} + \mathbf{u} \cdot \nabla \frac{\partial f_s}{\partial x} \right) + \dot{Q} \quad (1)$$

where $\Delta H$ is the latent heat of fusion, $\mathbf{u}$ is the velocity and $k_c$, $C_p$, and $\rho$ stand for effective thermal conductivity, effective specific heat capacity and density of the material, respectively. $f_s$ in this equation stands for solid volume fraction of the alloy, which is a function of temperature and varies in this study linearly with temperature over the solidification interval.

$\dot{Q}$ on the right-hand side of equation (1) is the volumetric heat generation term. Furthermore, this paper introduces mass-averaged thermal properties to determine the thermal conductivity and specific heat capacity of powder, which is:

$$C_p = \left[ \frac{1 - \varphi}{\rho_p \varphi + \rho_\text{sol} \varphi_\text{sol}} + \frac{\rho_p \varphi_\text{sol}}{1 - \varphi} \right]$$

where $\varphi$ is the initial volume fraction of powder, which is assumed to be 40% in this paper. For the case of 0% porosity, the effective thermal property would become the same as that of bulk material.

The mass and momentum balance equations for incompressible flow and Newtonian fluid are described as:

$$\nabla \cdot \mathbf{u} = 0 \quad (3)$$

$$\mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \mathbf{f}_{\text{c}} \quad (4)$$

in which the stresses $\tau_{ij}$ can be expressed as:

$$\tau_{ij} = -\frac{2}{3} \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + 2 \mu \delta_{ij} \frac{\partial u_i}{\partial t} \quad (5)$$

$F_{c}$ in (4) is a volumetric source term which is dependent on both fluid velocity and liquid fraction of the metal ($f_l$):

$$F_{c} = \frac{C(1-f_s)}{B + f_s} u_i \quad (6)$$

where $C$ and $B$ are constants that should be selected correctly to dissipate the velocities at the borders of the melt pool. The main phenomenon, which prompts the liquid metal to flow, is the Marangoni effect, which is related to the temperature gradient as:

$$\tau_{ij} = -\left( \nabla \sigma_{\text{surf}} \right) \frac{\partial T}{\partial t} \quad (7)$$

where $\nabla \sigma_{\text{surf}}$ is the surface temperature gradient and $\frac{\partial T}{\partial t}$ is the rate of change of surface tension with respect to temperature. Accordingly, positive values of this parameter will result in radially outward flow, while negative values lead to radially inward flow.

2.1 Microstructural model

As mentioned earlier, the microstructural model used for the subsequent heat treatment is an in house developed cellular automata (CA). The state transformation rule is the following for the CA used in this work is the following [10]:

- **If any** of the cells in the neighbourhood of the current cell has a state “1” change state of the current cell to “1”
- **If all** the cells in the neighbourhood have a state “1”, change the status of the current cell to “2” [11].

For the particular CA used here, three states are identified:

“0” is the untransformed state ($\alpha$), “1” is a cell, which is partially transformed, and “2” is the state of a cell that has finished its transformation ($\beta$).
It is clear from the previous explanation that the choice of the neighbourhood is important for the resulting microstructure. There are two neighbourhoods presented in Fig. 1: Moore and Neumann. Here, a combination of the two is used [14], which will be called the modified Neumann neighbourhood. The cells labelled with the number one are captured before the cells labelled with a number 2. This leads to rounder, more realistic grains.

The choice of neighbourhood can be reduced by including the growth velocity [11]. This also has the added benefit that it couples the CA time steps to the real time step. The basic CA algorithm is not time dependent, since it simply captures one cell per time step. Therefore, the CA used here takes into account the growth velocity as a function of temperature. A cell will only be captured when the velocity multiplied by the time step is larger than the diameter of a cell. For SLM, the growth velocity is obtained from the thermal and fluid-dynamics models. For the heat treatment, the empirical relation obtained by Semiatin et al. is used [13]. This equation is as follows:

\[ D - D_0 = k_0 E_a(T) r^n \]  

(8)

Here, \( D \) and \( D_0 \) are the final and initial diameter of the grains, \( t \) is time, \( n \) is the exponent which takes into account dimensionality, \( E_a(T) \) is a temperature dependent activation energy term, and \( k_0 \) is a proportionality factor. Finally, calculating the change in the nuclei density handles nucleation [11]. This change is integrated over the entire temperature range reached in this time step. The positions of the nuclei are chosen randomly among the available nucleation sites.

![Fig. 1. Three neighbourhoods: Neumann, Moore and modified Neumann](image)

**3. Results and discussion**

The size of computational domain for the macro model is 3 mm by 1.5 mm by 1.5 mm. For the matter of simplicity, only half of the domain is considered by incorporating a symmetry boundary condition. The powder layer is assumed to be homogenous and uniformly distributed over the top surface in the macro model. The laser starts to scan the top surface of the domain with scanning speed of 220 mm/s. The laser power is 300 watt, and the laser beam radius is 100 \( \mu \)m. Time step and minimum mesh size are set to 1e-8 s and 10 \( \mu \)m, respectively. Fig. 2 shows temperature contours at different times. As time passes, not only does the melt pool grow in size in all directions (note that it grows in an allotropic pattern), but the shape of the melt pool becomes more egg-shaped as well. Also, the maximum temperature of the domain, which occurs at the middle of the melt pool, increases with time until it reaches a pseudo-steady condition, where the maximum temperature will remain almost constant till the end of the process.

An interesting observation is that the dominant mode of heat transfer changes during the course of the process. The mode of the heat transfer is quantified by a dimensionless parameter, the Peclet number, which is defined as the ratio of heat advection and heat conduction. This number explains that the mode of heat transfer inside the domain is transformed from conduction to advection. The contours of velocity magnitude along with the velocity arrows at four different times are gathered in Fig. 3. Based on Fig. 3, as the laser moves, the average velocity magnitude rises until it converges to a constant value. From this moment onwards, the convection mode of heat transfer will be dominant. To have a deeper understanding of the velocity and temperature fields inside the melt pool, two different profiles of the liquid phase are demonstrated in Fig. 4.

![Fig. 2. Temperature contour and melt pool shape at four different times.](image)

Due to the thermo-capillary shear stresses formed at the top surface, the liquid metal flow at the top of the melt pool is radially outward. Also it can be seen that the velocity on the border of the melt pool, where liquid is in contact with the mushy zone, is tangent to the melt pool surface. This will lead to return of the flow to the centre of the melt pool which consequently leads to formation of the circular flow patterns in both cross sections as can be seen in Fig 4 [7, 8]. It is worth mentioning, it is because of mentioned rotational flow patterns that the maximum temperature will not plunge to unrealistically high values, since due to the Marangoni effect, the hot molten metal is transferred to cooler site near the borders of melt pool, where it transfers heat to unaffected
solid zones. A metallurgical sub-model is developed and coupled to the thermo-fluid model, which can acquire the main three solidification parameters, namely temperature gradient, cooling rate and growth velocity. In this paper, the growth velocity is determined as the velocity of the fluid at the border of the melt pool and on the onset of solidification. The corresponding temperature gradient along with the captured growth velocities for this process are shown in Fig. 5. According to this Fig., the predicted grain morphology is entirely in the columnar region [15]. Based on this morphology map, a columnar microstructure is generated with an average grain diameter is 68 µm ± 10 µm, which is based on experimental observations [16]. Since the nucleation sites for these grains are chosen randomly along the bottom edge of the computational domain, ten different microstructures are used as input for the microstructural model. One of these columnar microstructures is displayed in Fig. 6a.

A small parametric study reveals that the values, which give the best results, are 7 µm²/s for \( k_0 \) and a value of 1.5 divided by the number of nucleation sites for the nucleation density.

![Velocity and temperature field of the melt pool for two different cross-sections](image)

**Fig. 4.** Velocity and temperature field of the melt pool for two different cross-sections at \( t=3 \) ms.

The analysis of the grain diameters uses the line diameter as a measure of the actual grain size. This technique counts the number of grain diameters on lines drawn across the image. To obtain statistically relevant data, the heat treatment is modelled five times for each of the columnar microstructures, totalling 50 different simulated microstructures.

![Solidification map for the process](image)

**Fig. 5.** Solidification map for the process.

Fig. 6b shows one of these microstructures. The total size of the computational domain is 1.5*1.5 mm², and the cell size is 2 µm. It is visible that the grains are more equiaxed, similar to what is observed by Vrancken et al. [2], for a heat treatment of Ti64 at 1323 K for 1 hour.

![Histogram and fitted pdf for the measured grains](image)

**Fig. 6.** The initial (columnar) microstructure on the left (a) and the equiaxed microstructure after heat treatment on the right (b).

A histogram of the relative frequency of the simulated grain diameters is shown in Fig 7b. This histogram shows that the distribution of the measured grains is lognormal, and the shape is similar to experimentally measured line diameters. A fitted probability density function (pdf) reveals a mean of 287 µm for the simulated results with a standard deviation of 217 µm. This is comparable to the distribution, which is obtained from [16], where the grains have a mean of 296 µm and a standard deviation of 222 µm, shown in Fig. 7a.

![Empirical CDF](image)

**Fig. 7.** (a) Histogram and fitted pdf for the measured grains; (b) for the simulations, and (c), the cumulative distribution of frequencies for both.

In Fig. 7c, the cumulative distribution of frequencies (CDF) of the grains is also displayed for each of the simulations. The range of these CDFs gives an interval in which the experimental results should lie. The same experiments, which have been performed in an earlier study, are clearly contained within this range, although most of the simulations have slightly more smaller grains, which is also reflected in the average of the simulations, which is slightly smaller than the measured values.

### 4. Conclusion

In this paper, a thermo-fluid dynamic model is developed to model the temperature and fluid motion during SLM. The melt pool shape is evaluated and shows agreement with results found in literature. The fluid dynamic model shows the transition of the mode of heat transfer from conductive to advective. Next, the grain morphology of the as-produced part is evaluated using the growth velocity determined from the macro-model. Finally, the evolution of the microstructure is modelled using CA, and the simulations show good agreement with earlier reported experimental results. Future work will explore more complex fluid dynamics, and will aim...
to evaluate the mechanical properties of the SLM microstructure. Since this paper only looked at the martensite to beta transformation, future work will look into the beta to alpha transformation during cooling down.

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