Modeling of Phase Transformations and Internal Stresses in Laser Powder Deposition

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ABSTRACT

A finite element model coupling heat transfer calculations, phase transformations kinetics and internal stresses calculations to simulate laser powder deposition of a titanium alloy is presented. The model was applied to the study of the influence of the deposition parameters on the microstructure, hardness and residual stresses in Ti-6Al-4V thin walls produced by this method.

Keywords: Laser powder deposition, Ti-6Al-4V, phase transformations, modeling

1. INTRODUCTION

Laser powder deposition (LPD) is a rapid manufacturing technique whereby fully dense 3D parts can be produced directly from CAD models by overlapping consecutive layers of laser melted material. Being a CAD-based technique, LPD is very versatile in terms of the shape and size of the parts that can be manufactured and hence particularly well suited to the production of complex one-of-a-kind parts and repairing of worn out components [1-5].

During laser powder deposition, the overlapping of layers of material originates in the deposited material successive thermal cycles with a duration and amplitude which depend on the object geometry, build-up strategy used and processing parameters. These thermal cycles induce phase transformations in the material which may result in complex distributions of microstructure, residual stresses and properties that can drastically affect the performance of the components. Optimization of the build-up strategy is a costly and time consuming task, impractical to undertake experimentally, but it is well suited to a mathematical computational approach if a model is available which, by simulating the phase transformations caused by the heat and mass transfer phenomena that take place during fabrication, allows predicting the final microstructure, residual stresses and properties in the manufactured parts [6]. In this paper a three dimensional finite element thermo-kinetic-mechanical model that simulates laser powder deposition of Ti-6Al-4V is presented. The model is applied to investigate the influence of the deposition parameters on the microstructure, properties and residual stresses distributions in the deposited parts. The results achieved show that models of this type can be used to optimize the deposition process in order to achieve parts with enhanced properties and low residual stresses.

2. DESCRIPTION OF THE MODEL

The model is based on three sets of equations describing heat transfer, solid-state phase transformations kinetics in Ti-6Al-4V and deformation behavior, respectively. Solving the coupled set of equations for a complex shaped 3D part requires the use of numerical methods which entail discretization of both the space and time domains. In the model proposed, heat transfer calculations are carried out using the finite element method and use as input the material properties, part geometry and boundary conditions. The temperature variation at each point is used as input for a transformation kinetics subroutine that, taking into account the solidification structure, calculates the evolution of the material phase constitution due to the thermal cycles experienced during part build up. The calculated thermal field and microstructural evolution, together with the processing parameters and boundary conditions are then used as input for the thermal stress/strain calculations.

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2.1 Heat Transfer Calculations

The temperature distribution in the workpiece is calculated by solving the three dimensional heat conduction equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla (k \Delta T),$$  \hspace{1cm} (1)

where $\rho$, $c_p$ and $k$ are the density, specific heat and thermal conductivity of the material, all temperature dependent. Considering a Gaussian laser beam, the heat input due to the laser radiation is described by the surface heat flux:

$$Q_{\text{laser}}(x, y, t) = \alpha \frac{2P}{\pi r_1^2} \exp\left(-\frac{2x^2}{r_1^2}\right),$$  \hspace{1cm} (2)

where $\alpha$, $P$ and $r_1$ are the surface absorptivity, and the power and radius, respectively, of the laser beam. Heat losses by convection (Eq. 3) and radiation (Eq. 4) to the environment are accounted for as terms of the boundary conditions:

$$Q_{\text{convection}} = h(T - T_0),$$  \hspace{1cm} (3)

$$Q_{\text{radiation}} = \varepsilon\sigma(T^4 - T_0^4),$$  \hspace{1cm} (4)

where $T_0$, $h$, $\varepsilon$ and $\sigma$ are the room temperature, convective heat transfer coefficient, emissivity and Steffan-Boltzmann constant, respectively. The boundary condition takes the form:

$$k(\nabla T, n) = Q_{\text{convection}} + Q_{\text{radiation}} - Q_{\text{laser}}.$$  \hspace{1cm} (5)

Solving the heat transfer equation subjected to the above mentioned boundary conditions using the finite element method requires the part to be represented by a mesh that reflects as closely as possible its geometry. The equations describing heat transfer are then solved for each element in (ideally) infinitesimal time steps. Addition of material is taken into account by activating at each new time step elements with a volume corresponding to the volume of material deposited during the duration of that step. Taking into consideration the results of Neto and Vilar [7], which showed that in the blown powder laser deposition method the powder flying through the laser beam often reaches the liquidus temperature before impinging into the melt pool, the newly active elements are assumed to be at the liquidus temperature.

2.2 Modeling Solid-State Phase Transformations

Ti-6Al-4V is an $\alpha/\beta$ titanium alloy which presents two equilibrium phases, the hexagonal close-packed $\alpha$ phase and the body-centered cubic $\beta$ phase [8]. The proportions of the two phases in the alloy depend on the temperature and are given by [9]:

$$f_\beta(T) = \begin{cases} 0.075 + 0.92e^{-0.0085(980-T)}, & T < 980 \degree C \\ 1, & 980 \degree C \leq T < T_{\text{liquid}} \end{cases},$$

$$f_\alpha(T) = 1 - f_\beta(T).$$  \hspace{1cm} (6)

The phase transformations that can occur during deposition of this alloy are indicated in the diagram on Fig. 1.
1st Cycle

- Cooling from liquid
- \(\frac{dT}{dt} = 410 \, ^\circ C/s\)

2nd Cycle

- Re-heating
- \(\frac{dT}{dt} > 410 \, ^\circ C/s\)

Fig. 1 – Phase transformations in Ti-6Al-4V.

1st thermal cycle - Cooling from liquid

The solidification structure of Ti-6Al-4V consists of 100% \(\beta\) phase. During cooling to room temperature \(\beta\) may transform into two different phases, depending on the cooling rate (Fig. 1). If the cooling rate is lower than 410 °C/s, a diffusion controlled transformation will take place and the \(\beta\) phase will progressively transform to \(\alpha\) phase as it cools from 980 °C (known as the \(\beta\)-transus temperature) to room temperature. In isothermal condition the kinetics of this transformation is described by the Johnson-Mehl-Avrami (JMA) equation:

\[
f(t) = \left[1 - \exp\left(-kt^n\right)\right],
\]  

(7)

where \(f(t)\), \(k\) and \(n\) are the fraction transformed at time \(t\), the reaction rate constant and the Avrami exponent, respectively. The values for \(k\) and \(n\) were determined as a function of temperature by Malinov et al. [10]. Although the Johnson-Mehl-Avrami equation strictly applies to isothermal transformations, it can be generalized to anisothermal condition by the additivity rule, for example [11,12].

For cooling rates higher than 410 °C/s the \(\beta \rightarrow \alpha\) transformation is suppressed and \(\beta\) transforms by a martensitic transformation into \(\alpha'\) martensite. The proportion of \(\beta\) transformed into martensite depends essentially on the undercooling below the martensite start temperature (\(M_s\)) and is given by [13,14]:

\[
f_{\alpha'} = 1 - \exp\left[\gamma(M_s - T)\right],
\]  

(8)

The values of \(\gamma\), \(M_s\) and \(M_f\) used in the present work (0.015, 650 °C and 400 °C respectively) were calculated on the basis of the results of Elmer et al. [14].

2nd thermal cycle - Re-heating

When new layers of material are deposited, the material in previous layers is reheated. The heating/cooling cycle experienced at each point will induce solid state phase transformations which modify the microstructure and properties.
of the material. If the microstructure resulting from the first thermal cycle consists of \(\alpha + \beta\), reheating will cause the diffusional transformation of \(\alpha\) into \(\beta\), with a kinetics described by the JMA equation ((7). This transformation is the reverse of the transformation that occurred during cooling at rates lower than 410 °C/s (Fig. 1).

Heating up the martensite leads to its decomposition into the equilibrium proportions of \(\alpha\) and \(\beta\) when the tempering temperatures range is attained. This transformation occurs by a diffusional mechanism with a JMA kinetics. The values of \(k\) and \(n\) in (7 for the decomposition of martensite were determined by Mur et al. [15]. If the decomposition of martensite is incomplete, tempering results in a three-phase microstructure consisting of \(\alpha' + \alpha + \beta\).

2nd thermal cycle – Cooling

During cooling, martensite will continue to decompose into \(\alpha\) and \(\beta\). If cooling takes place at rates higher than 410 °C/s the \(\beta\) phase may undergo a martensitic transformation or be retained at room temperature depending on the volume fraction of this phase present in the alloy. Previous authors have observed that the \(\beta\) phase is retained upon quenching to room temperature if its volume fraction is lower than 0.25 [9,16,17]. If this volume fraction exceeds 0.25, a proportion of \(f_c = 0.25 - 0.25.f_\beta(T_0)\) will be retained at room temperature [17], where \(f_\beta(T_0)\) is the volume fraction of \(\beta\) prior to quenching. The remaining \(\beta\) \((f_\beta(T_0) - f_c)\) will undergo a martensitic transformation. Cooling of an alloy consisting only of \(\beta\) phase at rates higher than 410 °C/s originates a fully martensitic structure, while materials with smaller volume fractions of this phase retain a variable proportion of \(\beta\) at room temperature (Fig. 2). Thus, the martensite volume fraction is given by:

\[
f_\alpha(T) = f_\alpha'(T_0) + \left( f_\beta(T_0) - f_c \right) \left[ 1 - \exp\left( \gamma(M_s - T) \right) \right]
\]

where \(f_\alpha'(T_0)\) is the volume fraction of \(\alpha'\) prior to quenching. If the cooling rate is lower than 410 °C/s, \(\beta\) phase will transform into \(\alpha\) by a diffusional mechanism.

These phase transformations will continue during subsequent thermal cycles and the final microstructure will result from the transformation cycles at each point.

![Graph](image)

Fig. 2 – Phase constitution of Ti-6Al-4V at room temperature after quenching of an equilibrium microstructure as a function of the volume fraction of \(\beta\) phase before quenching, based on the results of Fan, Castro et al and Lee et al [9,16,17]. The maximum proportion of \(\beta\) is obtained by quenching from a composition with 0.25 \(\beta\), which is the equilibrium proportion of this phase at approximately 800 °C.

2.3 Calculation of Young’s Modulus and Hardness

The elastic modulus and hardness distributions in the part were calculated from the phase constitution of the alloy using the rule of mixtures [17]. \(\alpha\) and \(\alpha'\) present a similar elastic modulus, higher than the elastic modulus of \(\beta\) phase \((E = 117, 114\) and 82 GPa respectively), so the Young’s modulus will depend mainly on the proportion of \(\beta\) in the final structure.
The Rockwell hardness of $\alpha$, $\alpha'$ and $\beta$ is HRC = 30, 13 and 39 respectively [9]. The dependence of the hardness on the phase constitution of the final microstructure is shown in Fig. 3.

![Graph showing Young's modulus and Rockwell hardness (HRC) of Ti-6Al-4V as a function of the volume fraction of beta phase before quenching.]

Fig. 3 – Young’s modulus and Rockwell hardness (HRC) of Ti-6Al-4V as a function of the volume fraction of beta phase before quenching.

### 2.4 Yield Stress

During the deposition process, the thermal cycles experienced by the material will give rise to thermal expansion and contraction. Since the thermal history varies from point to point in the workpiece, the thermal expansion gradient will originate thermal stresses in the material. In laser processing these stresses are usually high enough to cause yield in some regions and, as a consequence, the final part will present residual stresses. The yield stress in Ti-Al-4V can be decomposed into the contributions of $\alpha$ and $\beta$ phases, the total yield stress being the weighted stresses of the individual phases in the microstructure [18,19]:

$$\sigma_y = \sum_{i=1}^{N} f_i \sigma_i,$$

where $f_i$ and $\sigma_i$ are the volume fraction and yield stress of the phase $i$, respectively. The constitutive expression for the yield stress of $\alpha$ phase is [18]:

$$\sigma_\alpha = K_\alpha \exp\left(\frac{273000}{RT_\alpha}\dot{\varepsilon}\right)^{1/4.6},$$

where $R$, $T$ and $\varepsilon$ are the gas constant, absolute temperature and strain rate respectively, and the coefficient $K_\alpha$ has the value 0.07. Similarly, for the $\beta$ phase we have:

$$\sigma_\beta = K_\beta \exp\left(\frac{160000}{RT_\beta}\dot{\varepsilon}\right)^{1/4.2},$$

with $K_\beta = 6.3$.

The von Mises yield criterion is used to determine the onset of yielding. This criterion states that yield takes place whenever the von Mises stress $\sigma_v$ exceeds the yield stress of the material (10):

$$\sigma_v = \sqrt{\frac{3}{2}} \sqrt{s_{ij} s_{ij}} > \sigma_y,$$

with $s_{ij}$ being the stress tensor components.
where $s_{ij}$ is the deviatoric part of the stress tensor $\sigma_{ij}$:

$$s_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij},$$

(14)

with $\delta_{ij}$ the Kronecker delta.

3. RESULTS AND DISCUSSION

The model was used to study the influence of the deposition parameters on the microstructure, hardness, Young’s modulus and residual stress distributions in Ti-6Al-4V walls (width = 0.50 mm; length = 2.50 mm; height = 1.25 mm) produced by overlapping 10 layers of Ti-6Al-4V using the same material as substrate. The deposition was assumed to take place in the midplane of the substrate, so that the problem is symmetrical in relation to this plane, and to reduce computational time only half of the geometry was considered (Fig. 4). The deposition parameters used in the simulation were: scanning speed = 2.5 mm/s, laser beam power = 725 W, laser beam radius = 1.5 mm, idle time between the deposition of consecutive layers = 1 s and initial substrate temperature = 27 °C. The distribution of phases along the wall height middle line is shown in Fig. 5, and the distribution of Young’s modulus and hardness in Fig. 6. The final part presents a non-uniform distribution of properties which is a consequence of the non-uniform microstructure in the deposited material. Close to the substrate and in the last layer, the material presents a fully martensitic ($\alpha'$) structure, while in mid-section of the wall the material consists of $\alpha'$ and retained $\beta$ (with a maximum of 16% $\beta$ phase and a minimum of 84% $\alpha'$ phase in the third layer). This non-uniform microstructure is the result of a thermal history that varies from point to point thus inducing different phase transformations at different points. Fig. 7 shows the temperature variation at the interface between the substrate and the wall during the buildup process. After the deposition of the first layer the temperature at the interface is about 250 ºC, and the deposited material undergoes a complete martensitic transformation upon cooling to this temperature. As new layers of material are added, the progressive heating up of the workpiece prevents the material deposited in the second, third and fourth layers from cooling down below $M_f$, and as a consequence the material in these layers will undergo an incomplete martensitic transformation. Tempering of the martensite ($\alpha' \rightarrow \beta + \alpha$) formed during the deposition of the first four layers takes place as the material is subjected to the successive heating/cooling cycles, but the intensity of tempering is small because the residence time of the material within the tempering temperature range (above $M_f$) during the complete deposition process (less than 10 s) is insufficient for significant martensite decomposition to occur. After the deposition of the last layer the workpiece cools down to room temperature. The material deposited in the fifth layer cools down from a fully $\beta$ phase structure, therefore it undergoes a complete martensitic transformation. The second to fourth layers are composed of $\alpha + \beta + \alpha'$, and after cooling some $\beta$ will be present in the microstructure at room temperature. The final part presents a mid-section where the hardness and the Young’s modulus are lower than in the upper and lower regions, due to the presence of retained $\beta$, which is softer and less stiff than $\alpha'$.

![Fig. 4 – Finite element mesh. If deposition takes place in the mid-plane of the substrate, a symmetry plane exists and the problem is solved in half the domain, taking a zero heat flux through that plane.](image-url)
Fig. 5 - Phase constitution along the wall height center line for an idle time of 1 s.

Fig. 6 – Distribution of Young’s modulus (top) and hardness (bottom) in the deposited part.

Fig. 7 – Temperature evolution at the interface between the substrate and the wall as a function of the layer deposited for two values of idle time: 1 and 60 s.
The residual stress distribution in the final part is shown in Fig. 8. The residual stress in the part does not exceed 200 MPa, much lower than the yield stress of Ti-6Al-4V at room temperature, 790MPa. The calculations show that deformation occurs predominantly at high temperature, and the plastic behavior of the material at these temperatures generates low residual stresses in the part.

Fig. 8 – Distribution of Von Mises stress, the upper limit of the scale is 790 MPa, which is the yield stress of Ti-6Al-4V at room temperature. The deformations are multiplied by a factor of 10.

Heating up of the workpiece during buildup is one of the main reasons for the non-uniform microstructure and properties distribution in the part. Heating of the substrate, in turn, is caused by the idle time between the deposition of consecutive layers being too short to allow sufficient cooling of the workpiece before the deposition of a new layer. Increasing the idle time will attenuate the substrate temperature rise, leading to different microstructure and properties. Using an idle time of 60 s while keeping all remaining parameters similar, the temperature at the interface between the substrate and the deposited material decreases below $M_f$ after the deposition of each layer (Fig. 7). This allows for a complete martensitic transformation to take place in all layers of material, leading to a part with a fully $\alpha'$ microstructure and uniform distribution of properties (Fig. 9 and Fig. 10).

Fig. 9 – Phase constitution along the wall height center line for an idle time of 1 s.
The residual stress distribution is plotted in Fig. 11. Once again, residual thermal stresses are lower than the room temperature yield stress of the material.

4. CONCLUSIONS

A thermo-kinetic-mechanical finite element model coupling heat transfer calculations, phase transformation kinetics theory and thermal stresses calculations was presented. This model allows predicting the microstructure, properties and residual stresses distribution in Ti-6Al-4V parts manufactured by laser powder deposition. Application of the model shows that:

- The final distribution of microstructure and properties in parts produced by laser powder deposition can be controlled by changing idle time between consecutive layers;
- Low idle times result in parts with gradients of microstructure and properties;
- A uniform microstructure with a high hardness can be obtained using high idle times;
- Residual stresses in the final part are approximately $\frac{1}{4}$ of the yield stress at room temperature;
- Mathematical-computational methods are effective tools for optimizing the laser powder deposition parameters and build up strategy, a task otherwise too costly and time consuming to be effectively carried out.

REFERENCES


