| Title          | Towards a process-structure model for Ti-6Al-4V during additive manufacturing |
|---------------|--------------------------------------------------------------------------------|
| Author(s)     | Yang, Xinyu; Barrett, Richard A.; Tong, Mingming; Harrison, Noel M.; Leen, Sean B. |
| Publication Date | 2020-12-15                                                                 |
| Publication Information | Yang, Xinyu, Barrett, Richard A., Tong, Mingming, Harrison, Noel M., & Leen, Sean B. (2021). Towards a process-structure model for Ti-6Al-4V during additive manufacturing. Journal of Manufacturing Processes, 61, 428-439. doi:https://doi.org/10.1016/j.jmapro.2020.11.033 |
| Publisher     | Elsevier                                                                     |
| Link to publisher's version | https://doi.org/10.1016/j.jmapro.2020.11.033                             |
| Item record   | http://hdl.handle.net/10379/16670                                           |
| DOI           | http://dx.doi.org/10.1016/j.jmapro.2020.11.033                              |
Towards a process-structure model for Ti-6Al-4V during additive manufacturing

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ARTICLE INFO

Keywords:
Additive manufacturing
Laser beam powder bed fusion
Microstructure

ABSTRACT

This paper presents the development of an integrated approach for microstructure prediction in laser beam powder bed fusion (PBF-LB) manufacturing of Ti-6Al-4V, primarily focused on the solidification morphology and solid-state phase transformation. A finite element (FE) model of the PBF-LB process is developed for prediction of thermal history and spatial distributions of temperature. Based on the relationships between FE predicted thermal history, thermal gradient and key manufacturing parameters such as laser power and scanning speed, an additive manufacturing (AM) process map for different solidification morphologies, including columnar-to-equiaxed transition, is developed. Phase transformation kinetics for the non-isothermal steps is adopted and implemented within a stand-alone code based on the FE predicted thermal histories of sample material points. The method is successfully validated by comparison with published experimental data and the developed process-structure model can be potentially used as a process design tool to efficiently produce tailored and optimized microstructures for specific applications.

1. Introduction

Additive manufacturing (AM) is an important technology for the manufacture of arbitrarily shaped and complex components, with the potential for more sustainable use of raw material, giving minimal non-recyclable waste, as compared to subtractive manufacturing methods [1]. AM of metal is characterized by a layer-by-layer deposition process and can be generally classified into two main categories: (i) powder bed fusion (PBF), in which a thin bed of powder is laid and the laser beam (LB) or electron beam (EB) melts the metal powder following a controlled trajectory, and (ii) directed energy deposition (DED), where the metal powder is coaxially fed into the beam and fuses with a thin layer previously deposited [2,3]. In this work, we focus mainly on the laser beam powder bed fusion (PBF-LB) process of Ti-6Al-4V. It is assumed that the metal powder is directly melted by the laser and subsequently solidifies during the cooling period. The platform is then lowered and applied with another thin layer of powder for subsequent laser melting. However, in contrast with solidification morphologies formed under equilibrium conditions, the complex heat transfer and molten metal flow during PBF-LB manufacturing has a significant effect on the thermal gradient and solidification rate, leading to quite different solidification morphologies and grain orientations [4–6]. At the same time, the complex thermal history will influence the microstructure formation through solid-state phase transformation [7].

Ti-6Al-4V alloy, due to its high specific strength, fatigue strength, corrosion resistance and biocompatibility, has been widely used for biomedical devices, as well as aerospace, marine and offshore applications [8,9]. There are two main crystal structures for Ti-6Al-4V: hexagonal close packed (HCP) \(\alpha\) phase and body centred cubic (BCC) \(\beta\) phase. The volume fraction of \(\beta\) phase is approximately 100% when the temperature is higher than the \(\beta\) transus point (\(T_{\beta}\), 994 °C [10]). Solid-state phase transformation from prior \(\beta\) to \(\alpha\) takes place during the continuous cooling process. The presence of vanadium and aluminium controls the transformation by diffusion and, hence, stabilizes the two-phase microstructure characteristic of Ti-6Al-4V [11]. Therefore, conventional Ti-6Al-4V has a \(\alpha\) phase fraction of approximately 80%–95% at room temperature, with the remainder being predominately \(\beta\) phase. However, the typically high cooling rates of \(10^3 \sim 10^8\) °C/s [12,
13] during the PBF-LB process result in a diffusionless transformation, and hence, a martensitic transformation when the temperature is cooled to the martensite start temperature ($M_s$, 575 °C [10]). This leads to the formation of a hierarchical martensitic microstructure [14–16]. Moreover, heat accumulation during successive depositions causes a bulk temperature increment, allowing for partial or complete martensite dissolution when the temperature is higher than the martensite dissolution temperature ($M_d$, 400 °C [17]). Thus, the thermal histories during PBF-LB are quite different from those of conventional casting or hot-working processes and will lead to a uniquely heterogeneous microstructure with different phase fractions, lath widths and displacement density throughout the material [18–22]. Depending on the cooling condition, Ti-6Al-4V has three different kinds of $\alpha$ phases: (i) grain boundary $\alpha$ ($\alpha_{gb}$), an allotriomorphic crystal structure located at prior $\beta$ grain boundaries; (ii) Widmanstätten $\alpha$ ($\alpha_w$), a lamellar structure which is usually aligned to form colonies and typically formed at slow cooling rates; and (iii) martensitic $\alpha$ ($\alpha'$), a needle-like structure which is a non-equilibrium phase formed at fast cooling rates.

This paper focuses on developing an integrated approach for simulation of the (i) thermal process, (ii) solidification morphology and (iii) solid-state phase transformation in PBF-LB processes. For the thermal process simulation, a finite element (FE) based solid-state model is adopted, where the powder bed is considered as a continuum body instead of individual particles. This has been shown to be a convenient and effective route to obtain detailed temperature field information [23–27]. Typically, Dai and Shaw [28] simulated the layer-by-layer process in PBF-LB by adding all the elements within one layer simultaneously onto the previous layer. Then a surface moving heat flux was coupled with the layer build-up approach to investigate the temperature gradient mechanism in PBF-LB of Ti-6Al-4V [29]. In contrast with previous work, a temperature-dependent powder absorptivity is incorporated in this paper and is shown below to give improved accuracy of melt pool size, for example, compared to previously-published results.

Solidification morphology, determined by the solidification process, significantly affects the mechanical properties [11,30]. Hunt [31] developed an analytical model for predicting transition from columnar-to-equiaxed grain structure. The Hunt model has been applied to various castings and laser glazes of Ti-6Al-4V for experimental verification [32]. Gockel et al. [33] presented the solidification morphology prediction of a single bead deposition in terms of two primary process variables, laser power and laser scanning speed, using a process mapping approach [34]. The two key thermal parameters associated with beam power and speed, respectively, are thermal gradient and solidification rate. However, a key limitation of this process-mapping approach for generating a power-speed map for real AM processes, which is addressed here, is the significant computational overhead required for finite element modelling of each combination of process variables. In this work, we adopt an alternative method, presented by Sheridan [35], based on the analytical Rosenthal solution [36], to avoid large amounts of inefficient and detailed computation.

After solidification, complex solid-state phase transformations between $\alpha$ and $\beta$ phases occur alternately during the heating and cooling cycles. Full-field and mean-field models, of different length-scales, can give detailed microstructural information but have considerable computational overheads. Therefore, an alternative approach, called the internal state variable approach [37] is more commonly used for phase transformation during welding and laser deposition [3]. The Kolmogorov-Johnson-Mehl-Avrami (KJMA) [38–40] nucleation and growth equation has been used to describe diffusion-controlled transformations (prior $\beta\rightarrow\alpha_{gb}$, $\alpha_w$) under isothermal conditions for Ti-6Al-4V [41]. Associated kinetic parameters for different $\alpha$ phases ($\alpha_{gb}$ and $\alpha_w$) were calculated from specific temperature-time-transformation (TTT) curves. For non-isothermal cooling processes, the KJMA equation has been discretized using the additivity rule [42,43]. On the other hand, the empirical Koistinen-Marburger equation [44] with a similar discretization logic has been employed for the formation of martensitic $\alpha$ (prior $\beta\rightarrow\alpha'$) due to its diffusionless process [18]. Martensite dissolution during heating cycles is a diffusional process, based on the current equilibrium volume fraction of $\alpha$ and $\beta$ phases [17], which can be described by the KJMA equation. The dissolution of $\alpha_{gb}$ and $\alpha_w$ combined with the growth of $\beta$ phase was modelled with an assumed parabolic rate law by Kelly [18], with application toDED processing of Ti-6Al-4V.

Based on the latter modelling developments, Charles and Jarvstrat [45] extended the modelling of welding deposition for Ti-6Al-4V to include $\alpha$ lath width prediction using an Arrhenius equation. Average $\alpha$ lath width is generally used as a characteristic length to assess the mechanical properties of lamellar Ti-6Al-4V, due to the strength increase being inversely proportional to $\alpha$ lath width. Charles et al. [14] further improved the formulations to present a comprehensive microstructural model for DED of Ti-6Al-4V. Irwin et al. [21] optimized the parameters in the Kelly–Charles model by experimental measurements of $\alpha$ lath width for Ti-6Al-4V, with martensite categorized as $\alpha$ phase to simplify the analysis. However, for the PBF-LB process, martensite plays a critical role and hence, needs to be specified as an independent variable. More recently, Yang et al. [22] predicted the martensite fractions for PBF-LB using a simplified kinetics model based on the carbon equivalent, which did not include the individual phase nucleation and growth, as addressed here.

In the present paper, an integrated approach for simulation from thermal process to the solidification morphology and solid-state phase transformation in the PBF-LB process for Ti-6Al-4V is developed. Firstly, a transient heat transfer simulation of the PBF-LB process is developed using the commercial FE software Abaqus®, to quantify the evolution of the thermal history and thermal gradient. Then, in order to predict solidification morphology, an analytical solution is combined with FE predicted results to generate a power-speed map for PBF-LB processing of Ti-6Al-4V, based on the Hunt criterion. Finally, the phase transformation model is formulated using the optimized parameters, and dedicated algorithms, accounting for the incomplete non-isothermal transformations during transient PBF-LB process.

2. Modelling method

2.1. Thermal process simulation

A three-dimensional layer-by-layer build-up model with a moving surface heat flux is implemented via a user subroutine to simulate the laser heating of the powder in PBF-LB process. The geometry and mesh are shown in Fig. 1. The part consists of two sections: the substrate and the powder bed. Five layers are built up for the powder bed with an individual (industry-standard) layer thickness of 30 μm. A mesh convergence study is conducted to establish a refined element size for the powder bed, with converged element size of 10 μm. The substrate is fixed at the bottom and the laser scans along the x-axis on the powder bed. 

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**Fig. 1.** Finite element model of substrate and part geometry for PBF-LB simulation.
bed surface. To simulate the layer-by-layer process, the analysis is divided into several steps in order to move the laser to successive layer surfaces after finishing the scanning of the previous step. At first, all the elements within the powder bed are deactivated. The first powder layer is then activated to simulate the first scan. When the laser moves to the next load step, the successive powder layer is activated and the previous load step is made inactive to account for the cooling cycle.

The moving heat flux is applied by a DFLUX subroutine in Abaqus®. A surface heat flux equation, including a 2D Gaussian distribution of specified surface intensity, powder absorptivity and laser spot radius, is assumed due to the minuscule layer thickness of powders [24, 29, 46]:

\[ I = \frac{2AP}{\pi r_0^2} \exp \left( -\frac{2r^2}{r_0^2} \right) \]

(1)

where \( I \) is laser intensity, \( A \) is powder absorptivity coefficient, \( P \) is laser power, \( r_0 \) is laser spot radius, and \( r \) is distance to laser beam center. Ti-6Al-4V powder absorptivity is modelled and experimentally validated by Boley et al. [47], as a temperature-dependent coefficient, expressed by:

\[ A(T) = \begin{cases} 
0.74 - 7.6 \times 10^{-5}T & 0 < T < T_v \\
0 & T > T_v 
\end{cases} \]

(2)

where \( T \) is the transient temperature in the PBF-LB process, \( T_v \) is the boiling temperature. The heat flux will be removed if evaporation takes place on the node, and the peak temperature is fixed at boiling point.

Table 1 summaries the PBF-LB manufacturing parameters for the experimental conditions investigated here, based on previously published work [48-51] and denoted as Samples I to IV. The hatch spacing is not considered here since attention is focused on the effects of primary process variables, such as laser power (\( P \)) and scanning speed (\( V \)) of the heat source. Fig. 2 shows the temperature-dependent thermal properties of specific heat and conductivity for Ti-6Al-4V powder and bulk materials. The phase transition temperatures and latent heat of Ti-6Al-4V are also considered in this simulation, as listed in Table 2.

### 2.2. Solidification morphology prediction

To predict the solidification morphology of PBF-LB Ti-6Al-4V, the solidification map based on the thermal conditions at the onset of solidification is used, as shown in Fig. 3, which was developed and experimentally validated by Kobryn et al. [52] for various casting and laser glaze cases. The thermal gradient at the solidification boundary, \( G \), is obtained using Fourier’s law [55]:

\[ |G| = |\nabla T| = \frac{|\mathbf{q}|}{k_L} \]

(3)

where \( |\mathbf{q}| \) is the magnitude of the heat flux vector and \( k_L \) is the thermal conductivity at the liquidus temperature. The solidification rate, \( R \), is determined via the solidification cooling rate \( S \) and thermal gradient \( G \):

\[ R = \frac{1}{|G|} \frac{dT}{dt} \]

(4)

The solidification cooling rate is:

Table 1

| Sample | \( P \) (W) | \( h \) (μm) | \( V \) (mm/s) | \( r_0 \) (μm) | Ref. |
|--------|------------|------------|-------------|-------------|-----|
| I      | 50         | 30         | 80          | 35          | [46]|
| II     | 20–80      | 30         | 200         | 26          | [49]|
| III    | 42         | 30         | 200         | 26          | [50]|
| IV     | 250        | 30         | 1600        | 26          | [51]|

\( P \), Laser beam power; \( h \), Layer thickness; \( V \), Laser scanning speed; \( r_0 \), Laser spot radius.

![Fig. 2. (a) Specific heat and (b) thermal conductivity of Ti-6Al-4V [49,52,53].](image)

![Table 2](image)

Table 2

| Parameter                                      | Value   | Reference |
|------------------------------------------------|---------|-----------|
| Solidus temperature, \( T_S \) (°C)            | 1605    | [52]      |
| Liquidus temperature, \( T_L \) (°C)           | 1655    | [52]      |
| Boiling temperature, \( T_b \) (°C)            | 3042    | [54]      |
| \( \beta \) transus temperature, \( T_{\beta} \) (°C) | 994     | [10]      |
| Martensite start temperature, \( M_s \) (°C)  | 575     | [10]      |
| Martensite dissolution temperature, \( M_d \) (°C) | 400     | [17]      |
| Latent heat, \( L \) (J/kg)                    | 365,000 | [52]      |

\[ \frac{dT}{dt} = \frac{T_L - T_S}{T_L - T_b} \]

(5)

where \( T_L \) and \( T_S \) are the liquidus and solidus temperatures reached at times \( t_L \) and \( t_S \), respectively.

As shown in Fig. 3, the solidification morphology is demarcated into three regions, namely fully columnar, fully equiaxed and mixed regions by the Hunt criterion boundary lines. Columnar grains grow in the direction of solidification, perpendicular to the substrate, while equiaxed grains are the preferred solidification structure with uniform dimensional distribution in all directions. A decrease in the \( G/R \) ratio corresponds to a transition of solidification morphology from planar to cellular columnar dendrite and eventually equiaxed grains [4]. The
of latent heat and temperature-dependent material properties, such as density, specific heat, thermal conductivity and powder absorptivity, by requiring only one FE simulation (i.e. one power-speed combination) to identify the calibration factor, as opposed to explicitly simulating a large number of power-speed combinations, to convert the solidification map (Fig. 3) into a power-speed process map (see below).

2.3. Solid-state phase transformation

Four solid-state phase transformation processes are modelled here, namely: (i) formation of \( \alpha_{gb} \) and \( \alpha_s \), (ii) formation of \( \alpha' \), (iii) dissolution of \( \alpha' \), and (iv) dissolution of \( \alpha_{gb} \) and \( \alpha_s \). A flowchart of the governing algorithm developed for this solid-state phase transformation between \( \alpha \) and \( \beta \) is shown in Fig. 5.

During the cooling process, \( \alpha_{gb} \) is firstly calculated due to its higher transformation rate at high temperature and then \( \alpha_s \) is updated. The remaining prior \( \beta \) phase fraction will transform to \( \alpha' \) if the cooling rate is fast enough and once \( M_i \) is achieved. During the heating process, \( \alpha' \) will dissolve into \( \alpha_s \) and \( \beta \) phases if the temperature exceeds \( M_i \). After that, \( \alpha_s \) and \( \alpha_{gb} \) will transform to \( \beta \) phase with increasing of temperature.

The KJMA model is usually used for the transformation between two phases during isothermal processes, where the initial phase at 100% will be transformed completely at infinite time:

\[
F = 1 - e^{-\beta(t_i)t_i^{n_i}}
\]  

where \( F \) is the fraction of formed phase, \( t_i^{eq} \) is the equilibrium time measured from the start of transformation and \( k \) and \( n \) are kinetic parameters which control the duration and the speed of the transformation. A modified KJMA model which can be applied for incomplete transformation and varying initial phase fractions is as follows [14]:

\[
F_n = \left[ 1 - e^{-\beta(t_i)t_i^{n_i}} \right] F_n^{eq} F_n^0
\]

where \( F_n \) is a phase fraction; \( F_n^{eq} \) is equilibrium a phase fraction (i.e., the fraction expected to remain after an infinite time at the current temperature), which is incorporated here to account for the incomplete transformation effect; \( F_n^0 \) is initial \( \beta \) phase fraction, considered for different initial phase fractions in different thermal cycles.

One of the challenges in modelling phase transformation for AM is the need to cater for non-isothermal conditions. Strictly, in a very rigorous, physically-based approach, it may be necessary to incorporate the effects of phase nucleation, nuclei growth and grain morphology. However, since the key objective of the present work is to develop a macro-scale approach for efficient, computationally-inexpensive prediction of the key microstructure parameters, a numerical approximation approach based on an additive rule [42,43] of the modified KJMA model is implemented, as illustrated in Fig. 6. The phase transformation is treated as a pseudo-fitting exercise using an isothermal KJMA solution at successive temperatures to update kinetic parameters. The thermal history is obtained from the FE-based thermal process simulation, with TTT curves for \( \alpha_{gb} \) and \( \alpha_s \) shown in Fig. 7. The 1% and 50% transformation curves are the most complete and available results obtained from the JMctlPro® calculation carried out by Kelly [18], and the effect of the initial and final phase fractions is considered when calculating the kinetic parameters. For a given time step \( t_i \), kinetic parameters \( k_i \) and \( n_i \) are obtained from an inverse calculation:

\[
n_i = \frac{\ln C}{\ln(t_i/t_{eq})}
\]

\[
k_i = -\ln(1 - F_i) t_i^{-n_i}
\]

\[
C = \frac{\ln(1 - F_i)}{\ln(1 - F_i^{eq})}
\]

where \( C \) is the characteristic parameter for reference TTT curves; \( t_{eq} \) and

thermal condition parameters, including thermal gradient and solidification rate, are calculated from the thermal process simulation and the solidification boundary is chosen as the trailing tip of the molten pool [34], which represents the first point during columnar-to-equiaxed transition, as shown schematically in Fig. 4. The trailing tip is therefore adopted in this paper as a representative point for a given set of process conditions. In order to generate a more industry-relevant process map for different laser powers (P) and scanning speeds (V), the analytical Rosenthal solution [36] is used to convert the solidification map to a power-speed map [35,56] using the laser power and scanning speed defined as:

\[
P = \frac{2\pi k_s (T_M - T_0)^2}{\Theta A G}
\]

\[
\frac{\partial T}{\partial t} = \frac{2\pi k_s V (T_M - T_0)^2}{\Theta A P}
\]

\[
V = \frac{1}{|G|} \frac{\partial T}{\partial t} = R
\]

where \( T_0 \) is the preheat temperature and \( \Theta \) is a calibration factor for the PBF-LB process, identified from FE simulation results using Eqs. (6) and (7). Eq. (6) shows the inverse relationship between laser power and thermal gradient, whereby higher laser power promotes more uniform heating through the layers, i.e. lower gradient. The solidification rate, as shown in Eq. (8), is equal to the scanning speed, consistent with the assumption that the molten pool is steady. It is worth nothing that this method significantly reduces the heavy computational overhead of detailed thermal process simulations with comprehensive consideration of
\( t_{i-1}, t_i \) are the start and final times of an isothermal transformation at a given temperature of \( T_i \) respectively; \( F_i \) is the initial phase fraction at \( t_{i-1} \), and \( F_{i+1} \) is the final phase fraction at \( t_i \). Therefore, the incremental form of Eq. (10) is:

\[
F_{\alpha,i} = \left( 1 - e^{-k(t_i-t_{i-1})} \right) \left[ F_{\alpha,i-1} \left( F_{\beta,i-1} + F_{\alpha,i-1} \right) \right] \tag{14}
\]
where the equilibrium time $t_0^{\alpha}$ can be calculated from:

$$t_0^{\alpha} = \left[ -\ln \left( 1 - \frac{F_{eq}^{\alpha}}{F_{gb,\alpha}} \right) \right]^{1/n_\alpha}$$

(15)

2.3.1. Formation of $\alpha_p$ and $\alpha_w$

The formation of $\alpha_p$ can be described by adapting the incremental formulation of Eqs. (14) and (15). Due to the difficulty of measuring the equilibrium fraction for $\alpha_p$ ($F_{eq}^{\alpha_p}$), $F_{eq}^{\alpha_p}$ is replaced by $F_{eq}^{\alpha}$ (as shown in Fig. 8) and $F_{gb,\alpha}$ is necessarily incorporated in the equation, due to the alteration from $F_{eq}^{\alpha_p}$ to $F_{eq}^{\alpha}$ [14]:

$$F_{\alpha_p,i} = \left[ 1 - e^{-b_{gb,\alpha} \left( \alpha_p^{eq} + \Delta \alpha_p \right)} \right] \left( F_{\alpha,i}^{eq} + F_{\alpha_u,i} + F_{\alpha_b,i} - F_{\alpha_g,i} \right)$$

(16)

The corresponding equilibrium time $t_0^{\alpha_p}$ is:

$$t_0^{\alpha_p,i} = \left[ -\ln \left( 1 - \frac{F_{\alpha_p,i} + F_{\alpha_g,i}}{F_{gb,\alpha} + F_{\alpha_g,i}} \right) \right]^{1/n_{gb,\alpha}}$$

(17)

Similarly, formation of $\alpha_u$ is expressed by:

$$F_{\alpha_u,i} = \left[ 1 - e^{-b_{gb,\alpha} \left( \alpha_u^{eq} + \Delta \alpha_u \right)} \right] \left( F_{\alpha,i}^{eq} + F_{\alpha_u,i} + F_{\alpha_b,i} - F_{\alpha_g,i} \right)$$

(18)

$$t_0^{\alpha_u,i} = \left[ -\ln \left( 1 - \frac{F_{\alpha_u,i} + F_{\alpha_g,i}}{F_{gb,\alpha} + F_{\alpha_g,i}} \right) \right]^{1/n_{gb,\alpha}}$$

(19)

2.3.2. Formation of $\alpha'$

The formation of $\alpha'$ is a temperature-dependent diffusionless process when the temperature is cooled below the martensite start temperature ($M_s$) with a high cooling rate. The empirical Koistinen–Marburger equation is used here to describe the non-equilibrium transformation:

$$F_{\alpha'} = \left[ 1 - e^{-b_{gb,\alpha'} \left( M_s - T \right)} \right] F_{\beta}$$

(20)

where $b_{gb,\alpha'}$ is a material parameter, taken as 0.005 from experimental work on Ti-6Al-4V [59].

According to the continuous cooling diagram [10], fully martensitic $\alpha$ forms if the cooling rate is larger than 410 °C/s, a block HCP $\alpha$, similar to that of the acicular martensitic $\alpha$ forms and is termed ‘massive’ $\alpha$ [10]. To simplify the modelling, ‘massive’ $\alpha$ is assumed to be the same as martensitic $\alpha$. Considering that the formation of ‘massive’ $\alpha$ is a diffusion-controlled process, the current equilibrium $\beta$ phase fraction is subtracted technically to avoid the fully martensitic transformation when the cooling rate is intermediate:

$$F_{\alpha',i} = \begin{cases} 
1 - e^{-b_{gb,\alpha'} \left( M_s - T \right)} \frac{F_{\alpha,i}^{eq} + F_{\alpha_u,i}}{F_{gb,\alpha}^{eq}} & \text{if } \dot{T} > 410 \text{ °C/s} \n1 - e^{-b_{gb,\alpha'} \left( M_s - T \right)} \frac{F_{\alpha,i}^{eq} + F_{\alpha_u,i}}{F_{gb,\alpha}^{eq}} & \text{if } 20 < \dot{T} < 410 \text{ °C/s}
\end{cases}$$

(21)

2.3.3. Dissolution of $\alpha'$

Dissolution of $\alpha'$ occurs during the heating period, leading to the formation of $\alpha_u$ and $\beta$ under a tempering-type effect. This dissolution is a diffusion-controlled process determined by the current equilibrium phase fraction [17]. The new $\alpha_u$ formed from the recovery of $\alpha'$ has a different crystallographic structure (i.e., lattice parameters) and composition to that formed from transformation of $\beta$, but this difference is not explicitly modelled [14]. The modelling method applied for the formation of $\alpha_p$ and $\alpha_u$ is also used here to describe the dissolution of $\alpha'$, and the dissolved $\alpha'$ is divided into $\alpha_u$ and $\beta$, referred to the current equilibrium phase fraction:

$$F_{\alpha',i} = F_{\alpha',i}^{eq} - \left[ \frac{F_{\alpha',i}^{eq} \left( C_{\alpha'} + \Delta \alpha' \right)}{F_{gb,\alpha'}} \right] \left( F_{\alpha',i}^{eq} + F_{\beta,i} - F_{\alpha',i}^{eq} \right)$$

(22)

$$F_{\alpha_u,i} = F_{\alpha_u,i}^{eq} + \left( F_{\alpha',i}^{eq} - F_{\alpha',i}^{eq} \right)$$

(23)

$$F_{\beta,i} = F_{\beta,i}^{eq} + \left( F_{\alpha',i}^{eq} - F_{\alpha',i}^{eq} \right)$$

(24)

where $F_{\alpha',i}^{eq}$ is equilibrium $\alpha'$ phase fraction, and $k_{gb}$ and $n_{gb}$ are temperature-dependent kinetic parameters, as defined in Table 3.

The corresponding equilibrium time $t_0^{\alpha'}$ is defined as:

| Temperature (°C) | $F_{\alpha'}^{eq}$ | $k_{gb}$ | $n_{gb}$ |
|-----------------|------------------|----------|----------|
| 400             | 0.75             | 1.019    | 0.667    |
| 500             | 0.20             | 1.015    | 1.106    |
| 700             | 0                | 1.025    | 1.252    |
| 800             | 0                | 1.031    | 1.326    |
\[ \theta_{\alpha i}^{eq} = \left[ -\ln \left(1 - \frac{F_{\alpha i+1} - F_{\alpha i}^{eq}}{F_{\beta i+1} - F_{\beta i}^{eq}} \right) / k_{\alpha i} \right]^{1/\nu_{\alpha i}} \]  \hspace{1cm} (25)

### 2.3.4. Dissolution of \( \alpha_g \) and \( \omega_w \)

Dissolution of \( \alpha_g \) and \( \omega_w \) leading to the growth of \( \beta \) phase has been represented mathematically by Kelly [18] as a parabolic rate \( r_{\beta i} \) (s \(^{-1/2}\)) based on ThermoCalc® and DicTra® calculations, where \( r_{\beta i} \) depends on the current temperature:

\[ F_{\beta i} = r_{\beta i}/\sqrt{t} \]  \hspace{1cm} (26)

\[ r_{\beta i} = a \left( \frac{K_i}{K_{\text{ref}}} \right)^b \]  \hspace{1cm} (27)

and \( K_i \) is the temperature in Kelvin and the reference temperature, \( K_{\text{ref}} \), is taken as 1 K here and used for dimensional consistency; the coefficient \( a = 2.2 \times 10^{-31} \) s \(^{-1/2}\) and the exponent \( b = 9.89 \) are adopted from Kelly [18]. The same approach for the incremental application of the modified KJMA model (Eq. (14) and (15)) is used here to introduce an equilibrium time \( \theta_{\beta i}^{eq} \):

\[ \theta_{\beta i}^{eq} = \left( \frac{F_{\beta i^{eq}}}{F_{\beta i}} \right)^2 \]  \hspace{1cm} (28)

In order to describe the extent of transformation, \( \Delta t + \theta_{\beta i}^{eq} \) is compared with \( (\theta_{\beta i})^{-2} \):

\[ F_{\beta i} = \left\{ \begin{array}{ll}
F_{\beta i}^{eq} r_{\beta i} / \sqrt{\Delta t + \theta_{\beta i}^{eq}} & \text{if } 0 < \Delta t + \theta_{\beta i}^{eq} < (r_{\beta i})^{-2} \\
F_{\beta i}^{eq} r_{\beta i} / \sqrt{\Delta t} & \text{if } (r_{\beta i})^{-2} < \Delta t + \theta_{\beta i}^{eq}
\end{array} \right. \]  \hspace{1cm} (29)

### 2.3.5. \( \alpha \) lath width prediction

The equilibrium value of \( \alpha \) lath width, \( w_{eqi} \), can be described by an Arrhenius equation following the approach of Charles and Jarvstrat [45], who studied the TIG metal deposition of Ti-6Al-4V:

\[ w_{eqi} = k_{w} \exp \left( -\frac{T_{act}}{T_i} \right) \]  \hspace{1cm} (30)

where the prefactor, \( k_{w} \), is 1.42 \( \mu \)m and the activation temperature, \( T_{act} \), is 20 °C, as also optimized by Irwin et al. [21] using simplex algorithms and further validated by Baykasoglu et al. [3] through scanning electron microscope (SEM). Lath width is assumed to depend on the total \( \alpha \) phase due to the primary \( \alpha \) and \( \beta \) kinetics [21]. Thus, the current \( \alpha \) lath width \( w_i \) is expressed as:

\[ w_i = \frac{1}{F_{\alpha i}} \{ w_{eqi} F_{\alpha i+1} + w_{eqi} (F_{\alpha i} - F_{\alpha i-1}) \} \]  \hspace{1cm} (31)

### 3. Results

#### 3.1. Temperature field

Fig. 9 shows a sample snapshot of the predicted temperature contours for the PBF-LB process for Sample I. The material with a temperature higher than the liquidus temperature is shown in grey, which indicates the molten pool. To validate the simulation result, the predicted thermal history for the selected point in the middle of the first laser track of Sample I is compared with corresponding test data measured by high speed thermography [48] for PBF-LB of Ti-6Al-4V. The thermal history presented in Fig. 10 corresponds to the deposition of three layers, showing three primary peaks in temperature. The scatter on the sample measured temperature data points is generally largest for the lower temperatures, due apparently to the effects of spattering of the molten metal [60]. It is clear that the FE predictions for the three peak temperatures, corresponding to the maximum heating from each track, are within a reasonable error range, with the largest prediction error of 3%. Furthermore, the heating and cooling rates, although not explicitly compared, are also captured reasonably well by the model. Besides these three primary peaks, several smaller peaks are measured, corresponding also to spattering [60]. In addition, the predicted molten pool dimensions in Sample II are compared to corresponding experimental data [49] and independent simulation results (Fu and Guo [29]) under the same PBF-LB conditions, as shown in Fig. 11. It is important to note that a temperature-dependent powder absorptivity is implemented here, in contrast to the constant value used in the previous simulation work [29]. Clearly, the present model, with temperature-dependent powder absorptivity, shows improved correlation with the measured data.

#### 3.2. Solidification morphology

Fig. 12(a) presents the predicted thermal gradient at the trailing tip of the molten pool in Sample I. A temperature decrease is predicted moving away from the trailing tip and the predicted temperature gradient is not as steep along the length (laser scanning direction) and width as in the depth direction. This is attributed to the heating of the powder in the depth direction by conduction, compared with direct laser radiation in other directions. The temperature field in the width direction is determined by the size of the beam, which is defined by a
Gaussian function in the DFLUX subroutine. As mentioned in the last section, the node in the middle of the first laser track of Sample I is selected to reveal the thermal history, as shown in Fig. 12(b). The peak temperatures represent the highest temperature for each heating-cooling cycle and are located in different regions, demarcated by the phase transition temperatures defined above in Table 2. The point experiences several thermal cycles and is melted during the first three cycles; the fifth layer deposition has a negligible thermal effect on the first layer. It is clear that the addition of layers and subsequent scanning is of primary importance to the previous layer and the cooling process takes only a small number of milliseconds from peak to near ambient temperature.

Using the prediction method developed in Section 2.2, the calibration factor, \( \varnothing \), is identified as 0.72 and the solidification map is converted to a power-speed solidification map for PBF-LB processing of Ti-6Al-4V, as shown in Fig. 13. Also shown (hollow dots on the figure) is the complete set of power-speed combinations identified as the optimized parameters for porosity-free as-manufactured material by Gong et al. [61], for PBF-LB of Ti-6Al-4V. It is clear that these cases are predicted to correspond to either fully columnar or mixed equiaxed-columnar. Furthermore, the process window from typical factory default settings (e.g. EOS M400) are also highlighted (dashed rectangle).

3.3. Phase fraction

As shown in Fig. 12(b), the PBF-LB process is characterized by extremely fast thermal cycles. Consequently, the experimental measurement of phase fraction evolution during this process is extremely challenging. Although one group have recently performed in-situ high-speed X-ray diffraction (XRD) for a single pulse [13] PBF-LB process on Ti-6Al-4V, unfortunately, measured phase fractions were not reported. Alternatively, the solid-state phase transformation model is validated here using data from the work of Babu et al. [62] for a DED process with
multiple layer deposition, including the thermal history, as input data, and the XRD result. Fig. 14(a) shows a comparison of the predicted total α phase fraction with the XRD test data as validation of the solid-state phase transformation model. It is clear that the model is in close agreement with the test data, with a difference between the prediction and experimental data of less than 2% for final phase fraction. The evolution of the different predicted α phase fractions is shown in Fig. 14 (b). Most of the α phase corresponds to α_w, while the phase fractions of α_g and α’ are both less than 5%.

Then the solid-state phase transformation model is applied with the PBF-LB process. The predicted phase fraction results for the PBF-LB process of Sample III are shown in Fig. 15. A key difference for the PBF-LB process is the dramatically shorter time-scales of the thermal cycles compared to the DED process, i.e. on the order of 10 milliseconds due to the more rapid laser scanning speed (as opposed to ~100 s for the DED process). This rapid cycling leads to a more complex microstructure than that of DED process, especially the large amount of martensite formed during the PBF-LB process. Fig. 15 also shows that the majority of martensite transforms to α_w and β, with negligible amounts of α_g. If the final heating-cooling cycle is applied with an optimized peak temperature. This transformation phenomenon is due to the effect of tempering treatment and the formed α_w is similar to tempered martensite (e.g. post-build heat treatment).

The phase transformation model developed here can also be used to predict the phase fractions after post-build heat treatment. As shown in Fig. 16, Ti-6Al-4V is almost fully martensitic in the as-printed state and transforms to α_w and β after heat treatment at 780 °C for 2 h and followed by furnace cooling. The result shows agreement with the SEM observations [51]. However, it is clear from Fig. 16(b) that the effective time for the transformation from α’ to α_w and β is much shorter than 2 h. This phenomena can be interpreted as a rapid tempering effect, an energy-saving manufacturing process with high tempering temperature and short duration (only about 1 s), which was introduced by Judge et al. [63].

3.4. α lath width

Fig. 17 shows the comparison of the predicted α lath width histories for Samples III and IV for the PBF-LB process. α lath width slightly decreases during the cooling process and different PBF-LB laser powers and scanning speeds lead to different α lath widths. As shown in Table 4, Sample IV has a much higher laser power and scanning speed, resulting in a narrower α lath at about 0.79 μm which is consistent with the experimentally-measured data of 0.85 ± 0.31 μm by Kaschel et al. [64]. Also, Kaschel et al. found that the α lath width decreases with laser power while the average Young’s modulus as well as ultimate tensile stress (UTS) show a positive correlation with laser power. Given that strength is inversely proportional to lath width [65], it can be deduced that higher laser power gives higher strength for PBF-LB Ti-6Al-4V.

4. Discussion

The present process-structure model offers a tool for simulation of the PBF-LB process. This includes thermal history to solidification, and associated solid-state phase transformations, to predict the salient microstructure attributes (e.g. columnar-equiaxed morphology, phase fractions, lath width) with the effects of different process parameters. To the authors’ knowledge, this is the first time such an integrated approach has been presented for PBF-LB process. Existing research tends
to focus on one or two aspects with specific process parameters, e.g. modelling of heat transfer and solidification microstructure \cite{4,66}, modelling of solid-state phase transformation \cite{7} and some RVE-based simulation using a phase field model for the grain growth and morphology prediction \cite{67,68}, which specifically contribute to a micro-scale analyses with onerous computational overheads.

In the thermal process simulation, the surface heat source is incorporated with a temperature-dependent powder absorptivity, which is shown to improve accuracy in prediction of molten pool dimension, when compared with previous similar work based on a constant powder absorptivity \cite{29}. The predicted thermal history, specifically including peak temperatures and cooling rate, is validated by comparison with the measured temperature by high speed thermography \cite{47}. It is found that the model captures the peak temperatures quite accurately, but slightly over-predicts the cooling rates (viz. $10^6$ $^\circ$C/s, as compared to $10^5$ $^\circ$C/s); however, this slight over-prediction is not significant with respect to prediction of prior beta to martensite phase transformation. More sophisticated modelling of the powder absorptivity, e.g. to include the different state (powder, liquid and solid) and inter-reflection among the powder particles \cite{69}, could potentially further improve predicted heating and cooling rates. At the same time, due to the omission of the flow of liquid metal, the convection of hot and cold fluids within the molten pool \cite{70}, the presence of surface-active elements altering the flow pattern of liquid metal \cite{71} and the effect of spattering \cite{60} are not explicitly considered here. Inclusion of these aspects would likely result in further improved model accuracy.

The solidification process map is based on the approach developed by Beuth et al. \cite{34} using the Hunt criterion and was modified to a more industrially-relevant power-speed map using the analytical Rosenthal solution to reduce the heavy computational overhead of the detailed thermal process simulation. According to the present map, fully equiaxed crystals, which are desirable for isotropic mechanical properties, are predicted to only occur at fast scanning speed and high laser power, due to the severe requirement for uniform solidification. This is consistent with previous reported observations \cite{66,72,73}.

Finally, the solid-state phase transformation is modelled by a numerical approximation approach using the modified KJMA equation and empirical Koistinen-Marburger equation. In contrast with the efforts contributed to the DED process \cite{3,14}, the present work managed to reveal corresponding phase transformations in reverse to capture the response to the complex heating-cooling cycle present in the PBF-LB process based on a 3D finite-element thermal simulation. As shown in Fig. 15, a large amount of $\alpha'$ appeared during the PBF-LB process because of the high cooling rate and portion of the martensite was dissolved in the final thermal cycle. Xu et al. \cite{74} verified this concept experimentally, demonstrating that the heat treatment time accumulated from the thermal cycling effect during PBF-LB is sufficient to lead to near-complete transformation of martensite into ultrafine lamellar ($\alpha$ + $\beta$), increasing both yield strength and elongation.

In particular, the $\alpha$ lath width prediction, validated by comparison with experimentally-measured data (Table 4) \cite{66}, was incorporated into the phase transformation model to predict $\alpha$ lath width, which can be further used to predict dislocation density, and hence, mechanical

\begin{table}[h]
\centering
\caption{Validation of $\alpha$ lath width prediction.}
\begin{tabular}{lccc}
\hline
Sample & Predicted value & Measured value & Reference \\
\hline
IV & 0.79 & 0.85 ± 0.31 & \cite{64} \\
\hline
\end{tabular}
\end{table}

Fig. 16. (a) Predicted breakdown of $\alpha$ phase and $\beta$ phase fraction for the PBF-LB process of Sample IV, and (b) with a post-build heat treatment at 780 $^\circ$C for 2 h followed by furnace cooling.

Fig. 17. Predicted $\alpha$ lath width for the PBF-LB process (a) Sample III, and (b) Sample IV.
5. Conclusions

This paper presents a process-structure model for laser beam powder bed fusion of Ti-6Al-4V; key conclusions are as follows:

- The method has been validated against previously reported measurements of thermal history, molten pool dimensions, solidification morphology, phase transformations and α lath width.
- The incorporation of temperature-dependent powder absorptivity improves accuracy in thermal process simulations, improving accuracy of predicted molten pool dimensions.
- The thermal gradient in the depth direction is significantly higher than in the width and laser scanning directions due to different heating efficiencies between thermal conduction and direct laser radiation.
- Laser beam powder bed fusion processes are predicted to form columnar or mixed crystals in general. This is consistent with previously-published findings.
- The evolution of solid-state phase transformation is predicted based on computed thermal history. The associated evolution of different phase fractions are thus predicted. It is shown that a large amount of martensitic α is generated during the laser beam powder bed fusion process, again consistent with previously published findings.
- It is possible to identify an ideal thermal history through control of the manufacturing parameters, to assist the in-situ decomposition of martensitic α, and hence create strong and ductile Ti-6Al-4V.

The present process-structure model is a key building block for development of a process-structure-property predictive methodology for PBF-LB processing of Ti-6Al-4V, which, in turn, will facilitate tailored manufacture of AM materials and components for improved mechanical performance, e.g. fatigue, fracture and tribology, particularly in critical applications, such as biomedical and aerospace.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This publication has emanated from research supported in part by a research grant from Science Foundation Ireland (SFI) under grant number 16/R3/3872 and is co-funded under the European Regional Development Fund and by I-Form industry partners. X Yang would also like to acknowledge helpful discussions with Frederico Kaschel and Prof. Denis Dowling, within the SFI I-Form Research Centre for Advanced Manufacturing in Ireland.

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