

**AN INTEGRATED PROCESS–STRUCTURE–
PROPERTY–PERFORMANCE MODELLING
FRAMEWORK FOR ADDITIVE LAYER
MANUFACTURING OF Ti-6Al-4V**

by

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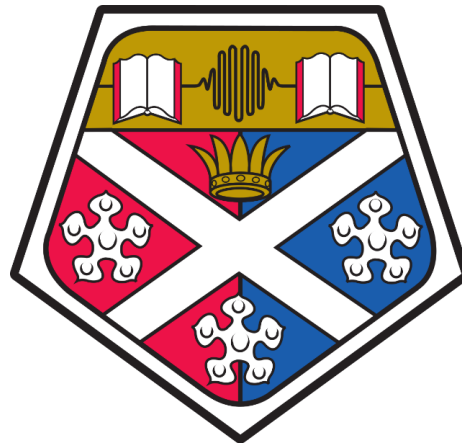
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Dedicated with love and gratitude to my family, friends and partner

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ABSTRACT

Additive Manufacturing is proving to be a revolutionary manufacturing process that is making its way into all engineering industries that require high-performance and light-weight structural components. This is mainly thanks to its ability to manufacture complex shapes that are unobtainable by conventional processes, which allows designers to be freed from manufacturing constraints and produce previously unmanufacturable components with unprecedented capabilities.

Nonetheless, the fast adoption of additive manufacturing is hindered by poor or inconsistent material performance that is highly dependent on a component's shape and manufacturing parameters. Computational models that establish relationships between geometry, process parameters, and performance offer a valuable solution to overcome this challenge. Such models can predict potential performance issues and guide the selection of optimal manufacturing parameters to prevent them. Nevertheless, developing these models is a complex task due to the intricate physics involved at different scales that impact the mechanical properties of an additively manufactured metal.

This Ph.D. thesis proposes a multi-physics and multi-scale modelling approach to fully digitally correlate the process parameters of selective laser melted Ti-6Al-4V with its elasto-plastic mechanical properties and structural performance. The method involves coupling micro-scale crystal plasticity simulations to calculate mechanical properties with a component-scale thermal process model through a mean-field microstructure evolution model. The developed automated modelling tool could be used in optimisation of process parameters and geometrical design to achieve peak performance in additively manufactured structural components.

Furthermore, a rigorous analysis of the developed model is presented with comprehensive experimental validation. Overall, the proposed Process-Structure-Property-Performance framework demonstrated a strong foundation for improving the predictive accuracy of digital structural analysis of additively manufactured components. However, several limitations were appreciated. The high computational cost of the thermal process model restricts its practicality for iterative optimisation frameworks, while the absence of damage and distortion modelling constrains its predictive scope. Addressing these challenges will be essential to extend the applicability of the framework and enable its integration into robust, industry-ready digital design and optimisation workflows.

1. INTRODUCTION

Additive manufacturing (AM) of metallic components has been proven to offer enormous potential to manufacture complex geometries in shorter time and lower cost compared to conventional manufacturing methods. Nonetheless, AM components might suffer from undesirable and non-homogeneous microstructural features; and hence subpar mechanical properties, whose occurrence is closely tied to the manufacturing process parameters used [1, 2].

Some of the advantages of AM over conventional manufacturing methods are, (i) it enables the fabrication of intricate shapes such as internal cooling channels and lattice structures [3], (ii) it allows to build several components of an assembly and even assemble them in the same print, (iii) it has no tool cost associated with prototyping, and (iv) it allows to produce a prototype directly from a CAD model with a single manufacturing process, among others.

However, AM also presents certain drawbacks, with the most significant one being the challenge of ensuring material quality in terms of porosity [4], surface finish [5], dimensional control [6], and mechanical properties [7]. Achieving the required high-quality standards of the industries where it has more potential, like aerospace or medicine, often requires additional post-processing techniques. This prevents AM from becoming the near net-shape single step manufacturing process that it aspires to be.

As can be seen in Figure 1 from ref. [8], even in a small cube of 5 mm length, widely different microstructures can form according to the local temperature history along the printed component. These different microstructures will lead to significant differences in mechanical properties like tensile strength, and variable performance in service leading to unpredictable resistance to creep, fatigue, and more.

Accurate prediction of these microstructures, along with their associated mechanical properties, would greatly facilitate the design process of additively manufactured components by ensuring that their structural performance meets expectations. Moreover, this predictive capability would enable to simultaneously tune the component geometry and process parameters to tailor the local microstructure for specific tasks, thereby achieving exceptional efficiency.

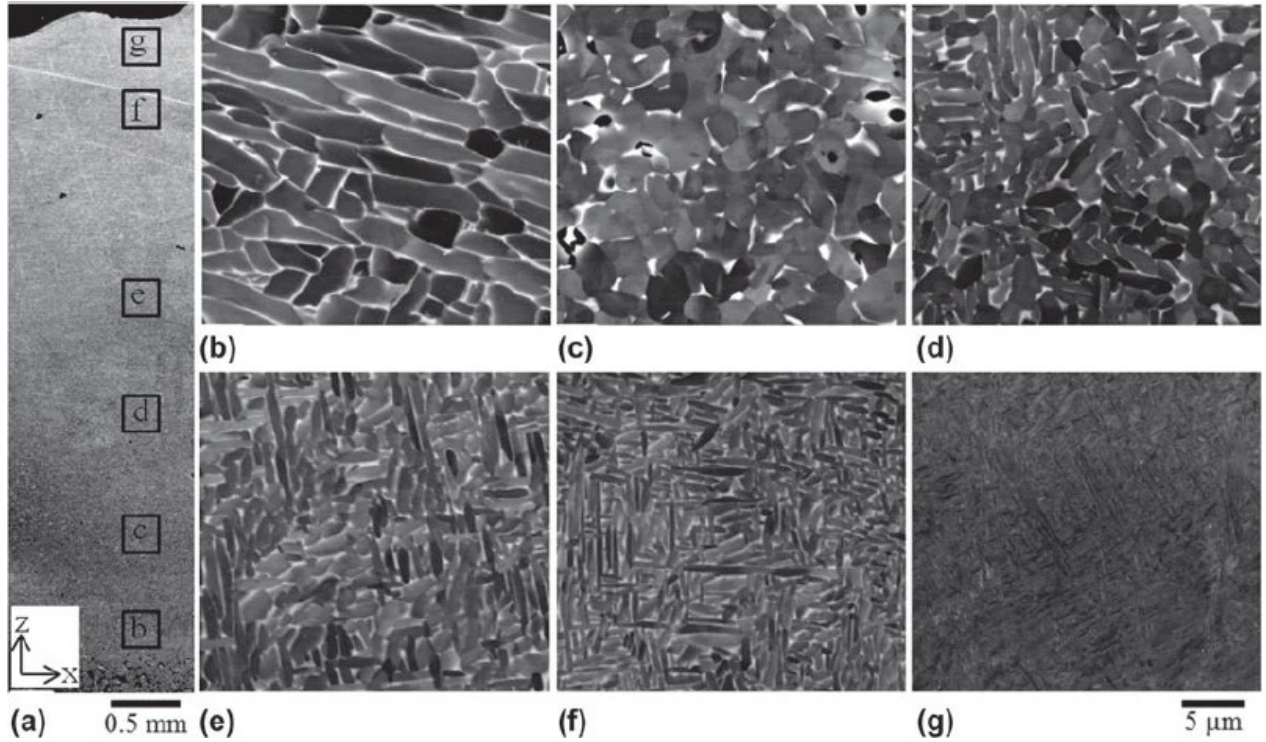


Figure 1. Images of different microstructures that form in the cross-section of a 5 mm cubic sample during laser powder bed fusion of Ti-6Al-4V. **a)** The different regions of a component from which the micrographs are taken, **b)** lamellar primary α , **c)** equiaxed primary α , **d)**, **e)**, **f)** bimodal, and **g)** martensitic α' . Reproduced from ref. [8].

The work in this thesis presents a computational framework for evaluating the intricate relationships between process parameters, microstructure, elasto-plastic properties and performance of additively manufactured Ti-6Al-4V (Ti-6Al-4V) components using Laser Powder Bed Fusion (LPBF) processes. The developed framework employs a multi-scale modelling approach to capture the influence of process parameters on local elasto-plastic mechanical properties. The obtained local mechanical properties can then be used in Finite Element Analysis (FEA) models to assess the structural performance of a component, yielding a Process-Structure-Property-Performance (PSPP) model.

The reader must note this work focuses on modelling fully dense and stress-free components, ignoring important defects like porosity, residual stress and surface roughness. Although these defects have significant influence on mechanical performance and would certainly need to be predicted in a full digital twin of the AM process, it is not feasible to develop a model that combines all of these effects in a single Ph.D. studentship. Instead, the developed models predict solely the

effects of “perfect” microstructures on mechanical properties, focusing on the effects of different grain sizes and phase fractions, which is a more reasonable objective. Furthermore, only static elasto-plastic tensile properties have been predicted, which are not enough to characterize performance in components subjected to creep or fatigue. Nonetheless, the reader will find several suggestions throughout the thesis of how these models could be extended to overcome these limitations and possibly achieve a full digital twin of AM.

The developed modelling approach, summarized in Figure 2, begins with a component-scale thermal model that calculates local temperature histories during the whole additive manufacturing process. This information is then utilised in a mean-field microstructural evolution model, which calculates the local phase fractions and grain morphology throughout the component. This approach yields the key microstructural information in different regions of the modelled components.

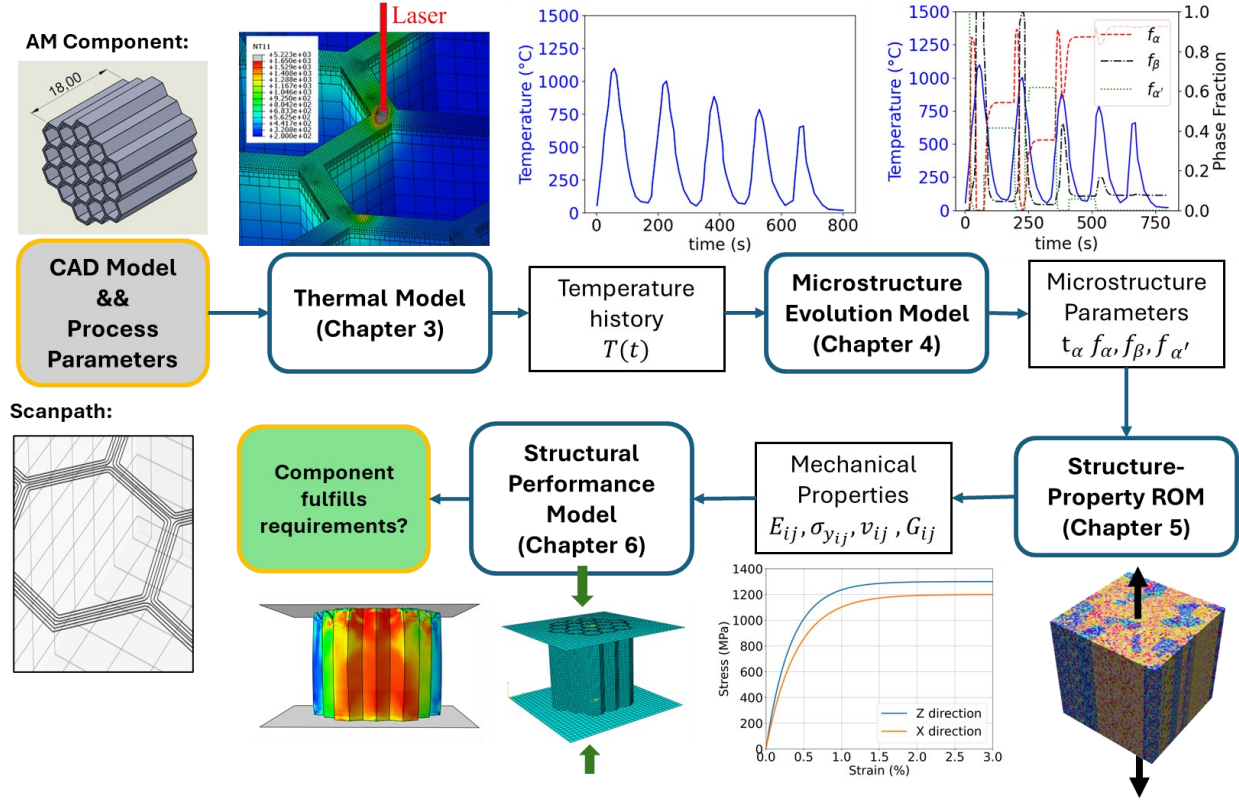


Figure 2. Schematic representation of the developed PSPP framework, showing an example for a 3D printed honeycomb. The diagram illustrates how a structural FEA model with spatially resolved mechanical properties is generated from the input CAD geometry and process parameters. This is achieved through a thermal FEA model that provides local temperature histories, a microstructure evolution model that predicts the resulting local microstructure, and a crystal plasticity Reduced Order Model (ROM) that determines the corresponding local mechanical properties.

Then, to evaluate the mechanical properties associated with each microstructure, a micro-mechanics Crystal Plasticity (CP) model is employed. CP enables the calculation of mechanical properties considering the previously calculated microstructural features by numerically solving a boundary value problem on a digital representation of a small, microscopic region of the material. The obtained local mechanical properties from the CP model are then integrated into macro-scale mechanical FEA models to assess the structural performance of the final component against a specific design load.

By incorporating the local mechanical properties into the macro-scale FEA models, the structural response of the additively manufactured component under design load can be effectively

quantified. This ensures that the component exhibits an appropriate structural behaviour, meeting the desired performance requirements.

1.1 Aims and Objectives

The objective of this work is to develop a simulation tool that offers mechanical designers and manufacturing engineers the ability to optimise the performance of components considering microstructure evolution during AM. To achieve this, this thesis aims to address the following research questions:

- Can local temperatures during additive manufacturing be predicted with enough accuracy for microstructure evolution predictions?
- Can the local variations in microstructure that arise from metal additive manufacturing be predicted?
- Can the tensile elasto-plastic properties associated with each potential microstructure be predicted?
- Can these predictions effectively assist in the engineering and manufacturing of structural components?

In this thesis, these questions will be answered for the case of LPBF of Ti-6Al-4V, for which a PSPP prototype model will be created for a honeycomb lattice structure. Although these questions have been previously studied for other materials and simpler AM processes, to the knowledge of the author they have not clearly resolved for a method with the complex thermal history of LPBF and the intricate structure-property relations of Ti-6Al-4V. This additive manufacturing method is widely used for high-performance metal components, and Ti-6Al-4V is one of the most commonly 3D printed alloys. Meanwhile, it is worth noting that with minor adjustments, the developed methodology can be extended to other materials and additive manufacturing processes. Also, other materials might even be simpler to model since Ti-6Al-4V is composed of a multi-scale dual phase microstructure with complex process-structure-property relations.

By addressing these research questions, this PhD thesis aims to provide the groundwork for a valuable automatic simulation tool that enables designers and engineers to optimise component performance through enhanced understanding and control of microstructural variations and associated mechanical properties. This will contribute to advancing the field of additive

manufacturing and facilitate the development of high-quality and functional components across various industries.

1.2 Structure of the Thesis

The main body of the thesis commences with a comprehensive literature review (**Chapter 2 - Literature Review**) used to elucidate the need for Process-Structure-Property-Performance (PSPP) models in additive manufacturing of Ti-6Al-4V and analyse the most prevalent modelling tools and already existing PSPP models in the literature. It also explains how the review leads into the chosen PSPP modelling methodology.

Since the developed PSPP simulation is composed of 4 different models that can also be used independently of each other, the explanation of the methodology of the PSPP modelling approach and their experimental validation has been divided into 4 different chapters. Each of these chapters covers a single model of the PSPP chain and contains its own modelling and experimental validation methodology sections, together with a discussion of its accuracy and possible areas of improvement. **Chapter 3 - Thermal FEA Model of LPBF for the prediction of Phase Transformations**, focuses on thermal modelling of the powder bed fusion process to calculate local temperature histories. Next, **Chapter 4 - Microstructure Evolution Model of Ti-6Al-4V**, dives into the prediction of microstructural features during the process from a known temperature shistory. Afterwards, **Chapter 5 - Microstructure-Property Modelling of Additively Manufactured Ti-6Al-4V**, details how CPFE can be used to relate microstructural features to mechanical tensile properties. Finally, **Chapter 6 - Process-Structure-Property-Performance Modelling of Additively Manufactured Ti-6Al-4V**, explains how local property prediction can be combined with a mechanical FEA model at the macro-scale to assess the structural performance of an AM component against a design load, while considering microstructural heterogeneity. The connection between the different modelling chapters is illustrated in Figure 2.

Finally, a conclusions section is presented (**Chapter 7 - Conclusions**) with a strong emphasis on possible areas of future work on how to further develop the model for increased accuracy, speed and the calculation of other relevant properties.

2. LITERATURE REVIEW

The following review analyses the need for holistic modelling in the design of additively manufactured Ti-6Al-4V components and explores the main approaches proposed to achieve this goal. It begins by examining the common challenges related to material quality in additive manufacturing. This is followed by an in-depth discussion of the effects of additive manufacturing on the microstructure of Ti-6Al-4V and a comparison with conventional processing routes. The review then surveys the state of the art in modelling tools for additive manufacturing, with particular attention to their applicability and limitations. Finally, the insights gathered are synthesised to justify the modelling strategy adopted in this thesis.

2.1 Material Quality in Additive Manufacturing and the need for Material Modelling

It is widely recognised that manufacturing defects and inconsistent material quality pose significant challenges in metal additive manufacturing [9-11]. These obstacles can greatly impact the quality and performance of additively manufactured components. Common manufacturing defects include voids, porosity, poor surface finish, distortion, and residual stress. Even in the absence of these defects, additively manufactured components often exhibit inferior mechanical properties compared to conventionally manufactured counterparts. These deficiencies encompass anisotropy, undesired and heterogeneous microstructures, low creep and fatigue resistance, and reduced ductility; which are primarily attributed to the complex thermal history experienced during the additive manufacturing process [12].

While post-processing techniques such as heat treatments or hot isostatic pressing (HIP) can mitigate some of these effects, they are often expensive and time-consuming [13, 14]. Consequently, achieving desirable properties in additive manufacturing components necessitates precise adjustment of process parameters for each specific material and component. This requires a thorough understanding of metallurgical thermodynamics during the additive process. Moreover, the multitude of process parameters, including geometry, laser power, and scanning speed, further complicates the task of developing effective parameter settings. Relying solely on experimental

trial and error to optimise these parameters is impractical due to the extensive time and resources required.

Therefore, addressing these challenges and avoiding undesirable effects in additive manufacturing components necessitates a comprehensive approach that combines fundamental knowledge of its thermodynamics with advanced modelling and optimisation techniques [15]. By leveraging computational simulations and models, it becomes possible to gain insights into the complex interactions between process parameters, material properties, and component performance. This enables the development of efficient and robust process parameter settings, ultimately enhancing the quality and performance of additively manufactured components while reducing the reliance on costly and time-consuming post-processing methods.

2.2 Microstructure and Properties of Laser Powder Bed Fused Ti-6Al-4V

2.2.1 Titanium and its alloys

Titanium (Ti) is a transition metal of significant industrial importance, distinguished by its combination of low density (4.51 g/cm^3), high strength, and excellent corrosion resistance. These attributes give titanium one of the highest specific strengths among structural metals, making it particularly attractive in applications where weight reduction is critical. Titanium also exhibits outstanding resistance to oxidation and to aggressive environments such as chlorides, seawater, and biological fluids, which further broadens its technological relevance [16].

The family of titanium alloys extends the usefulness of the pure metal by incorporating carefully selected alloying elements to enhance strength, toughness, and processing characteristics. This versatility has led to widespread adoption in multiple sectors, some of which are displayed in Figure 3. In aerospace, titanium alloys are essential for both airframe and engine components, where their strength-to-weight ratio and thermal stability improve performance and fuel efficiency. In the biomedical field, titanium's natural biocompatibility, combined with its corrosion resistance to bodily fluids, has established it as the material of choice for load-bearing implants and prosthetics. In addition, titanium alloys play an important role in marine structures, chemical processing equipment, and energy systems, where their ability to resist corrosion translates into longer service life and reduced maintenance costs [17].

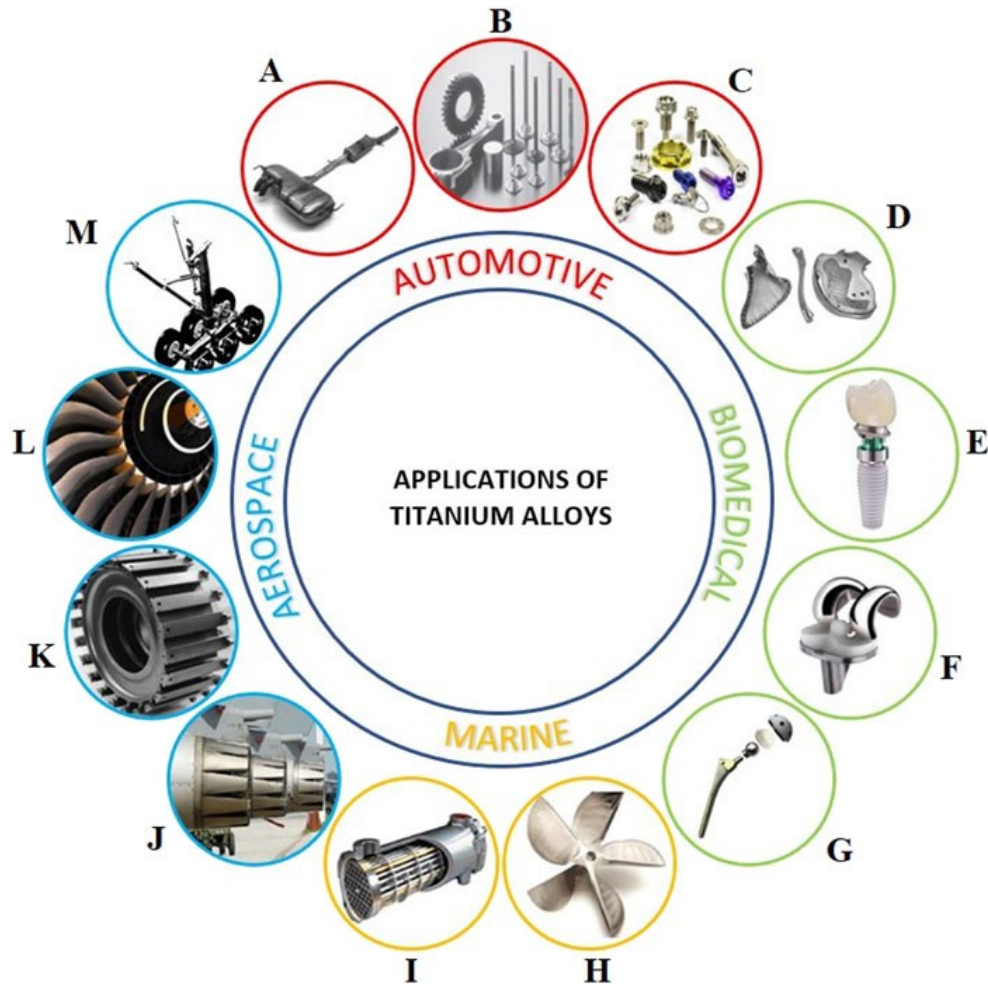


Figure 3. Example applications of Ti and its alloys. In automotive A) exhaust, B) engine parts, and C) fasteners; biomedical: D) complex implants, E) dental implant, F) knee implant, G) hip implant; marine: H) propeller, I) heat exchanger; aerospace: J) exhaust nozzle, K) fan disk, L) fan blades, M) main landing gear. Reproduced from [17].

Despite their advantages, titanium and its alloys also face certain limitations that have influenced their industrial uptake. High production and processing costs, relatively poor machinability, and sensitivity to impurities restrict their wider use compared to steels or aluminum alloys. Nevertheless, continuing developments in extraction, processing, and advanced manufacturing techniques, such as powder metallurgy and additive manufacturing, are gradually overcoming these challenges. This sustained progress ensures titanium and its alloys remain at the forefront of advanced materials research and engineering innovation.

2.2.2 Phases and Phase Transformations in Ti-6Al-4V

α and β

The metallurgy of pure Ti is dominated by the allotropic crystallographic transformation at 882 °C, called the β -transus temperature, at which the α phase transforms to β . Below this temperature, its equilibrium crystal structure has a Hexagonal Closed Packed (HCP) structure known as α and above β -transus it is a Body Centered Cubic (BCC) called β . The main effect of alloying this material (i.e., mixing with additional elements) is the shift of its transformation temperatures, which also allows to yield a two-phase material with both α and β present concurrently. Elements with extensive solubility in α (e.g., Al, O, N, C, Ga) will increase the β -transus temperature and are called α stabilisers. Vice-versa, elements with high solubility in β (e.g., V, Mo, Nb, Ta, Cr, etc) decrease it and are called β stabilisers. The effect of different alloying elements on the β -transus can be seen in Figure 4.

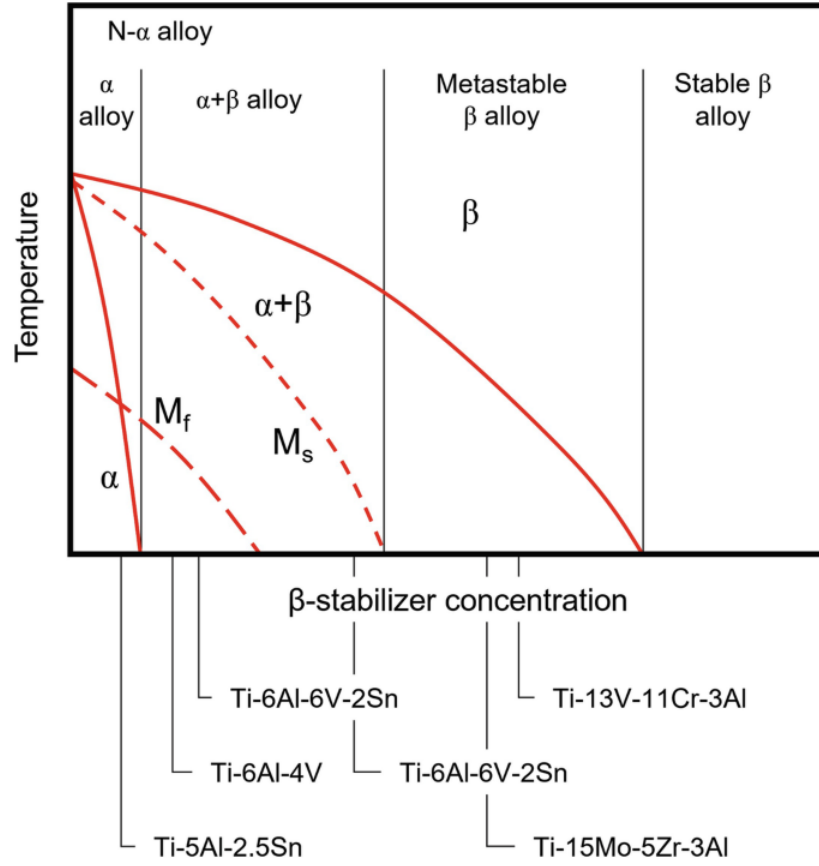


Figure 4. Schematic phase diagram showing the effect on transformation temperatures of adding β stabilisers to a near- α (N- α) Titanium alloy. With no β stabilisers, the alloy will contain only α at room temperature. As the amount of β stabiliser concentration is increased, the amount of β at room temperature increases. M_s and M_f denote the start and finish of the martensitic transformation, which happens during fast cooling rates. Image reproduced from ref. [18].

Regarding their mechanical properties, β tends to be more ductile than α due to a higher number of active slip systems in BCC systems than in HCP lattices. The slip directions of HCP and BCC crystals are displayed in Figure 5 and Figure 6, respectively. The elastic modulus of β is also lower in contrast to α . For these reasons, α is referred to as the hard phase and β as the soft phase.

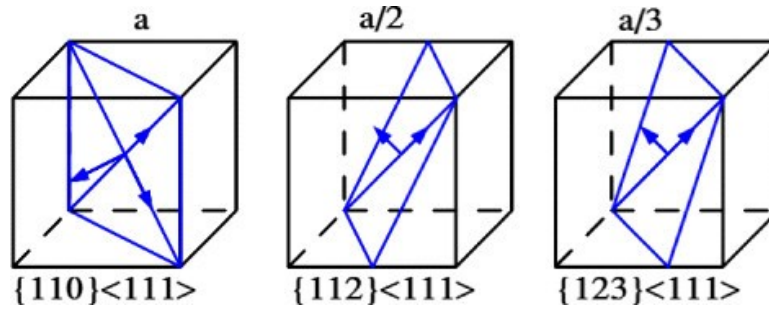


Figure 5. Slip systems of the Body-Centered-Cubic (BCC) crystal lattice. Reproduced from ref. [19]. The $[20]\langle 111 \rangle$ and $[13]\langle 111 \rangle$ systems have 12 variants each, while the $[13]\langle 111 \rangle$ has 14 variants.

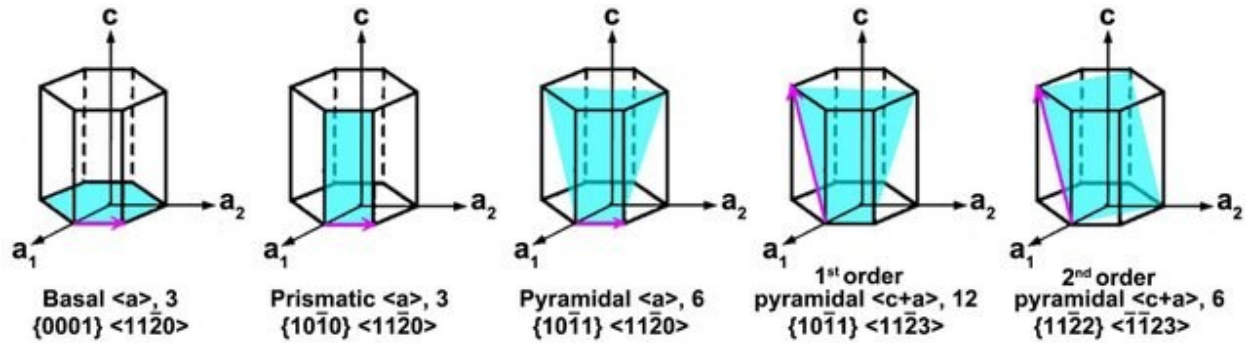


Figure 6. Slip systems of the Hexagonal-Close-Packed (HCP) crystal lattice. Reproduced from ref. [21].

Based on their phase constitution, Ti alloys are generally classified into the following 4 categories:

- **α alloys** (e.g., Ti-5Al-2.5Sn): stabilised primarily by α -stabilizers such as Al, O, or Sn. They exhibit good creep resistance and oxidation resistance at elevated temperatures, but relatively limited strength and poor formability. They are often used in aerospace gas turbines and high-temperature components.
- **Near α alloys** (e.g., Ti-6Al-2Sn-4Zr-2Mo, Ti-6Al-5Zr-0.5Mo-0.25Si): with small additions of β -stabilisers, they retain good high-temperature properties while offering better strength and toughness than pure α alloys. Their applications include compressor discs and blades in aeroengines.
- **$\alpha + \beta$ alloys** (e.g., Ti-6Al-4V, Ti-6Al-2Sn-4Zr-6Mo, Ti-6Al-7Nb): these alloys combine balanced properties due to the coexistence of both phases. They offer high strength, moderate fracture toughness, good fatigue resistance, and biocompatibility, making it dominant in aerospace structures, biomedical implants, and marine components.

- **Metastable β and near- β alloys** (e.g., Ti-10V-2Fe-3Al, Ti-15Mo, Ti-15V-3Cr-3Sn-3Al [Ti-15-3], Ti-5Al-5Mo-5V-3Cr [Ti-5553]): stabilised by β -stabilisers such as Mo, V, Cr, or Nb. These alloys can be solution-treated and aged to achieve very high strengths (>1200 MPa) and good formability. They are increasingly considered for airframe applications, fasteners, and springs. Some β alloys, such as Ti-35Nb-7Zr-5Ta, are specifically designed for biomedical use due to their low elastic modulus and excellent corrosion resistance.

The material of focus in this thesis, Ti-6Al-4V, is an α - β titanium alloy. This means that it contains both α and β stabilising elements, which are Al and V respectively. This alloy composition leads to a room temperature microstructure that usually contains a mixture of α (> 90%) and β ($\approx$ 8%) phases, where each phase has a high composition of their stabilising elements, meaning that α has a high composition of Al and β is rich in V.

Martensitic α'

Besides α and β , if the cooling from β -transus is fast, with a cooling rate higher than 410 °C/s, a non-equilibrium metastable martensitic phase called α' forms by a displacive transformation. Displacive or diffusionless transformations are solid-state transformations that happen without atomic diffusion. In these transformations, atoms displace distances smaller than the crystal's atomic spacing. For the case of Ti-6Al-4V, during fast cooling the BCC β transforms to an HCP phase by shear-dominated transformations. It yields a supersaturated solid solution enriched with Vanadium [22, 23], because it is not able to diffuse into a Vanadium rich β matrix like in diffusional transformations. For this reason, martensitic regions show little to no BCC β phase. Its crystal structure is an HCP lattice structure similar to α but with a slightly larger unit cell and c/a ratio. However, most importantly, it is characterised by numerous stacking faults substructures [24], high number of dislocations, nano-twins and high microstrain [25]. With such a highly distorted lattice, α' is stronger but relatively more brittle than its equilibrium counterpart α [26]. It is also believed that this microstructure produces subpar fatigue resistance [27], although the effect of martensite phase fraction on ductility and fatigue is still a matter of ongoing study [23]. This is because martensite is usually removed during the conventional thermomechanical processing of Ti-6Al-4V. However, it is of interest for AM methods, where it is more prominent in the final material due to the high cooling rates inherent to these processes.

Since it is a metastable phase, holding an α' microstructure at high temperatures will induce the decomposition of α' into a stable mixture of $\alpha + \beta$. Martensite decomposition is a diffusional process that takes place via nucleation and growth or spinodal modes [28]. During the decomposition of α' into α , vanadium is constantly rejected from the forming α and diffuse along accommodation twin boundaries or stacking faults towards the boundaries between adjacent α' plates. Discrete β particles will form along these α' plate boundaries and then continuously grow at the expense of vanadium until they connect at the fully decomposed α grain boundaries [24]. If the temperature is not held for long enough, partial decomposition may occur which leads to a mixture of α' , α and β whose phase fractions will depend on the thermal history. The atom probe tomography measurements from partially decomposed AM Ti-6Al-4V [24] allow to visualise a partial martensite decomposition, which is displayed in Figure 7. The elemental distributions show a matrix of lower atomic density where the composition is similar to graded Ti-6Al-4V. Inside this matrix, regions of higher atomic density exist with lower amount of V and higher concentration of Al. The former corresponds to α' and the latter to α , and shows the nucleation and growth of α inside the α' plate. The lower atomic density of α' is attributed to the large number of dislocations and stacking faults.

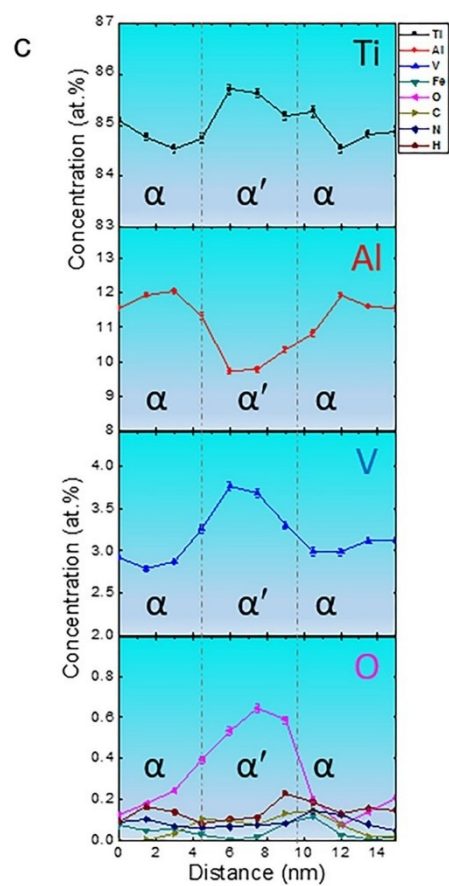
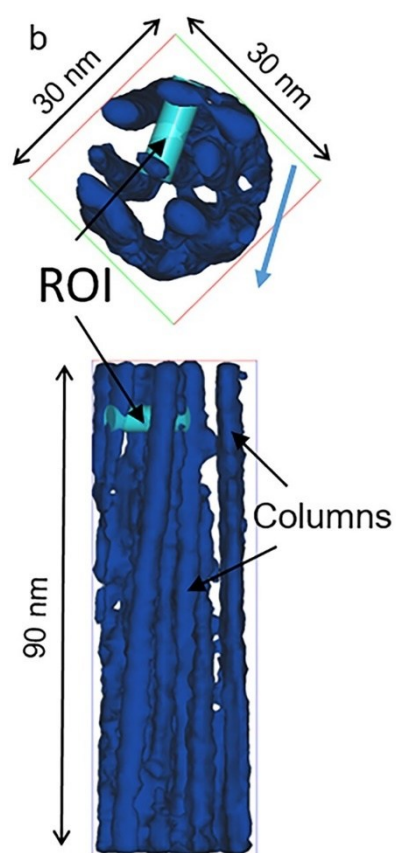
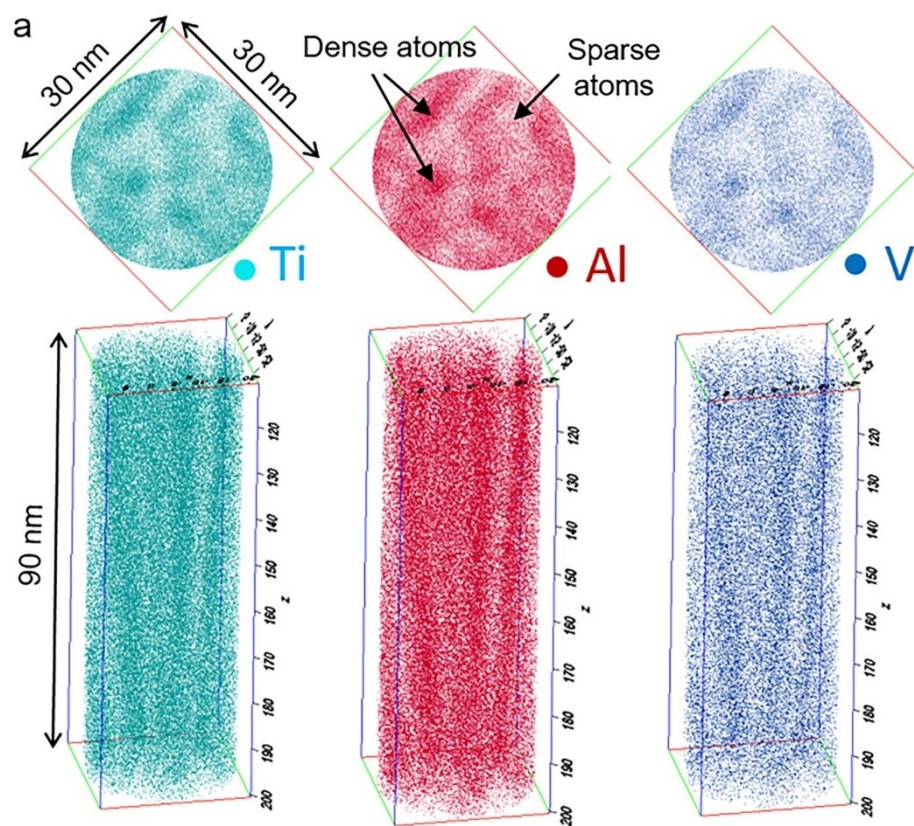


Figure 7. Atom probe tomography measurements in additively manufactured Ti-6Al-4V. **a)** Elemental distribution of Ti, Al and V from views of transverse and longitudinal directions. **b)** A cylindrical Region of Interest (ROI) that delineated with iso-density surfaces of $Ti + Al + V = 20 \text{ at. nm}^{-1}$. The columns of higher atomic density are indicated by arrows. **c)** 1D concentration profiles of all alloying elements in the ROI along the arrow direction indicated in b). As the dense atoms regions have very close compositions with initial Ti-6Al-4V ELI, they are determined to be martensite. Constrained α inside α' is confirmed, indicating martensitic formation and its partial decomposition from nanoscale. Images reproduced from ref. [24].

2.2.3 Microstructure Morphology in Ti-6Al-4V

Besides the relative fraction of α and β phases, the morphology of the microstructure is equally important in determining the mechanical properties and performance of titanium alloys. Even for the same chemical composition and phase balance, processing routes can produce very different morphologies such as equiaxed, lamellar, or bimodal structures, each associated with distinct deformation mechanisms. Lamellar microstructures (shown in Figure 8.a)), produced by slow cooling from the β phase field, constrain slip within α plates and impede its transfer across colony boundaries. Martensitic α' microstructures (shown in Figure 8.b)), generated by rapid quenching offer very high strength due to fine acicular α' plates, but they are usually brittle unless further aged. This gives higher fracture toughness and creep strength but can reduce fatigue performance. Equiaxed α grains (shown in Figure 8.d)) generally allow more uniform slip and dislocation motion across multiple grains, resulting in good ductility and high fatigue resistance. These examples highlight how morphology controls dislocation activity, crack initiation, and propagation, and therefore tunes the mechanical response as much as phase balance does.

Microstructural morphology can be modified through a combination of heat treatment and thermomechanical processing. For instance, working in the $\alpha + \beta$ field followed by controlled cooling yields equiaxed or bimodal structures, whereas cooling from the fully β region produces lamellar colonies. Heat treatment schedules, such as solution treatment and aging, further refine or coarsen the morphology, enabling property optimisation for different applications. This ability to engineer morphology gives titanium alloys a high degree of tunability, allowing the same alloy chemistry to serve in applications as diverse as high-cycle fatigue-sensitive aerospace structures or high-temperature creep-resistant turbine components.

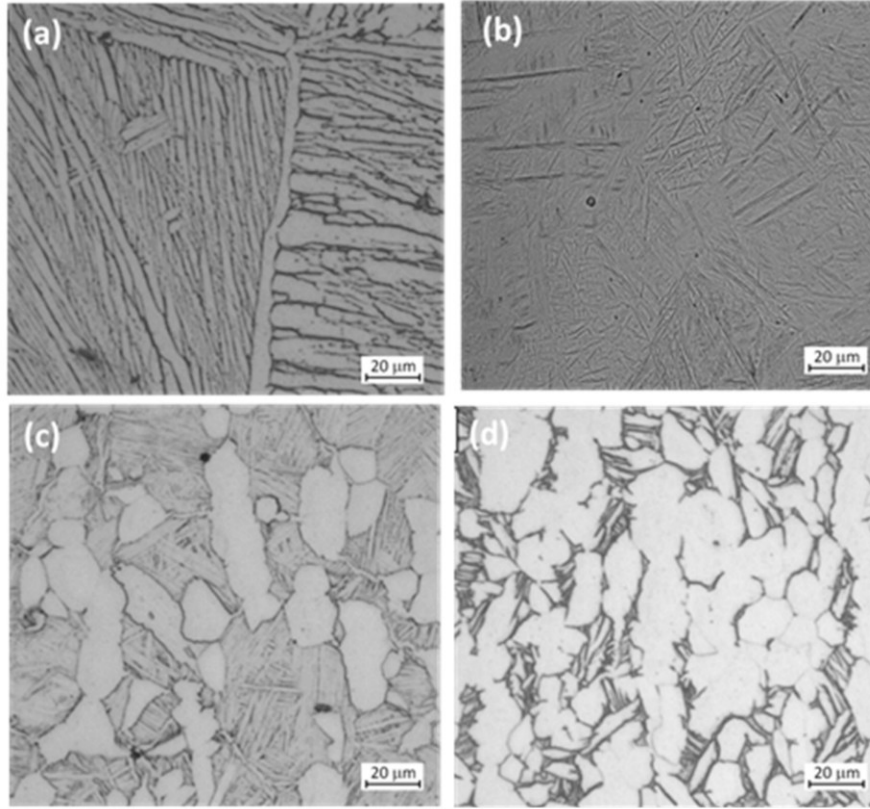


Figure 8. Different microstructures of Ti-6Al-4V alloy. **a)** Lamellar $\alpha + \beta$, **b)** martensitic α' , **c)** bimodal microstructure with globular α grains (white) and lamellar $\alpha + \beta$ from the prior β grain, and **d)** equiaxed α grains (white) and intergranular β at the α grain boundaries. Images reproduced from ref. [29].

2.2.4 Microstructure and Properties in Wrought Ti-6Al-4V

In the case of Ti-6Al-4V, the most widely used titanium alloy, conventional processing is carefully designed to achieve a bimodal (or duplex) microstructure (shown in Figure 8.c)). The route typically involves ingot casting (i.e., double/triple Vacuum Induction Melting & Vacuum Arc Remelting) followed by extensive thermomechanical working such as forging and rolling at temperatures just above β -transus and/or in the $\alpha + \beta$ phase field. This deformation breaks up the β grains and promotes the formation of equiaxed primary α , while subsequent controlled cooling allows the remaining β to transform into lamellar α colonies. Final heat treatments, often a solution treatment in the $\alpha + \beta$ field followed by aging, are employed to refine the microstructure and stabilise the desired phase distribution. Figure 9 displays an example of processing route and images of the microstructures before and after such thermo-mechanical treatment. The example

shows the microstructure of the cast ingot, containing lamellar α inside large parent β grains. This microstructure is transformed to a bi-modal microstructure through several steps. Firstly, a homogenizing heat treatment is applied, which is a high-temperature hold applied to the ingot to reduce chemical and microstructural inhomogeneities. Then, the plastic deformation is applied at a temperature near β transus. Afterwards, a recrystallization annealing heat treatment is performed, which allows the equiaxed primary α to develop from the previously distorted and elongated α grains after the plastic deformation. Finally, stress can be relieved by a heat treatment at lower temperatures.

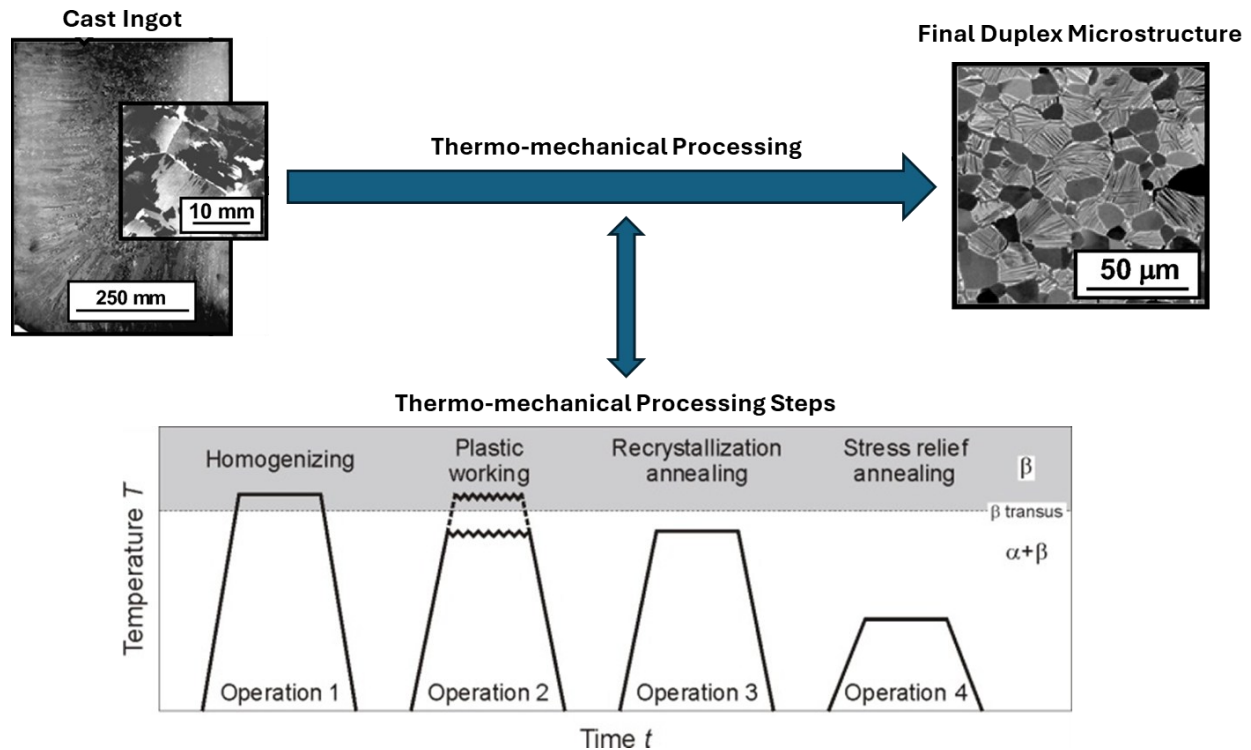


Figure 9. Schematic of conventional thermo-mechanical processing of Ti-6Al-4V. It starts with a cast-ingot, whose microstructure is shown. Through several of steps of heat treatments and hot plastic deformation, a duplex microstructure is achieved containing a combination of equiaxed α and lamellar $\alpha + \beta$. Images adapted from ref. [30, 31].

The resulting bimodal microstructure offers an excellent balance of mechanical properties. The equiaxed α grains provide pathways for homogeneous slip, enhancing ductility and fatigue resistance, while the lamellar regions contribute higher strength and toughness by impeding crack propagation and dislocation motion. This dual contribution makes bimodal Ti-6Al-4V exceptionally versatile, suitable for load-bearing aerospace components such as compressor blades

and structural airframe parts, as well as biomedical implants where a combination of strength, fatigue performance, and biocompatibility is required. The reproducibility of this bimodal morphology through conventional thermo-mechanical processing has been a key factor in Ti-6Al-4V's dominance across critical industries.

2.2.5 Microstructure and Properties of Additively Manufactured Ti-6Al-4V

As previously explained, Ti-6Al-4V possesses a high specific strength, good ductility, and excellent corrosion resistance make it a widely used alloy for relatively high temperature (i.e., up to 600 °C) structurally demanding applications such as light-weight components used in aeroengines [32]. Furthermore, it has a very good biocompatibility which makes it a highly demanded material for the biomedical industry [33]. These industries happen to be very interested in using AM for different reasons. On one hand, AM in automotive and aerospace industries can induce significant weight reductions and therefore increase performance due to the complex and highly efficient shapes that AM can produce, like lattice structures. On the other hand, AM allows to develop patient specific implants without having to tailor complex casting and subtractive manufacturing approaches for every patient. For these reasons and its good weldability, Ti-6Al-4V is the most 3D printed alloy today.

However, the effects of AM on Ti-6Al-4V can make its microstructure and properties significantly different than its conventional manufacturing counterparts. Forging allows to obtain a consistent bi-modal microstructure containing primary α grains produced by globularisation and lamellar secondary α grains in a β matrix [34, 35]. This microstructure has been proven to be very reliable in terms of toughness and fatigue life. On the other hand, AM of Ti-6Al-4V can produce different microstructures that depend on the geometry and process parameters used, which are hard to predict and can significantly affect structural performance.

During the solidification after melting inherent to the additive manufacturing process, Ti-6Al-4V tends to form long Parent β Grains (PBGs) that grow epitaxially and are highly elongated with a preferential growth in the building direction which typically leads to a strong $\langle 100 \rangle$ fibre texture. This texture is caused by the high thermal gradients and cooling rates experienced during the process, which cause grains whose (100) crystal orientation is aligned with the gradient to overgrow other grains [36]. These high thermal gradients and cooling rates are produced because AM usually melts a very small region of material in a much larger substrate, which acts like a heat

sink (i.e., conducts the heat away quickly), producing a temperature gradient in the BD [32]. With further cooling, the PBGs will transform into α' or α depending on the cooling rate. This final α/α' microstructure follows the Burger's Orientation Relationship (BOR) with respect to its PBGs, meaning that each α/α' lath inside a PBG can have one of the 12 possible orientations during $\beta \rightarrow \alpha$ phase transformation. This leads to the α/α' microstructure inheriting the high texture of the PBGs and producing anisotropic mechanical properties [37]. The EBSD inverse-polefigure (IPF) maps with respect to the vertical building direction of the final microstructure of a typical Ti-6Al-4V component, manufactured by AM, are presented in Figure 10, together with its polefigures (PF). They highlight the $\langle 100 \rangle$ fibre texture of the PBGs, i.e. most grains have their 100 crystallographic direction aligned with the BD, and how this leads to colonies of orientations in the final microstructure. This texture is a differentiating factor from conventional manufacturing, where the initial β can be better controlled to avoid strong textures, and the final component does not show anisotropic properties.

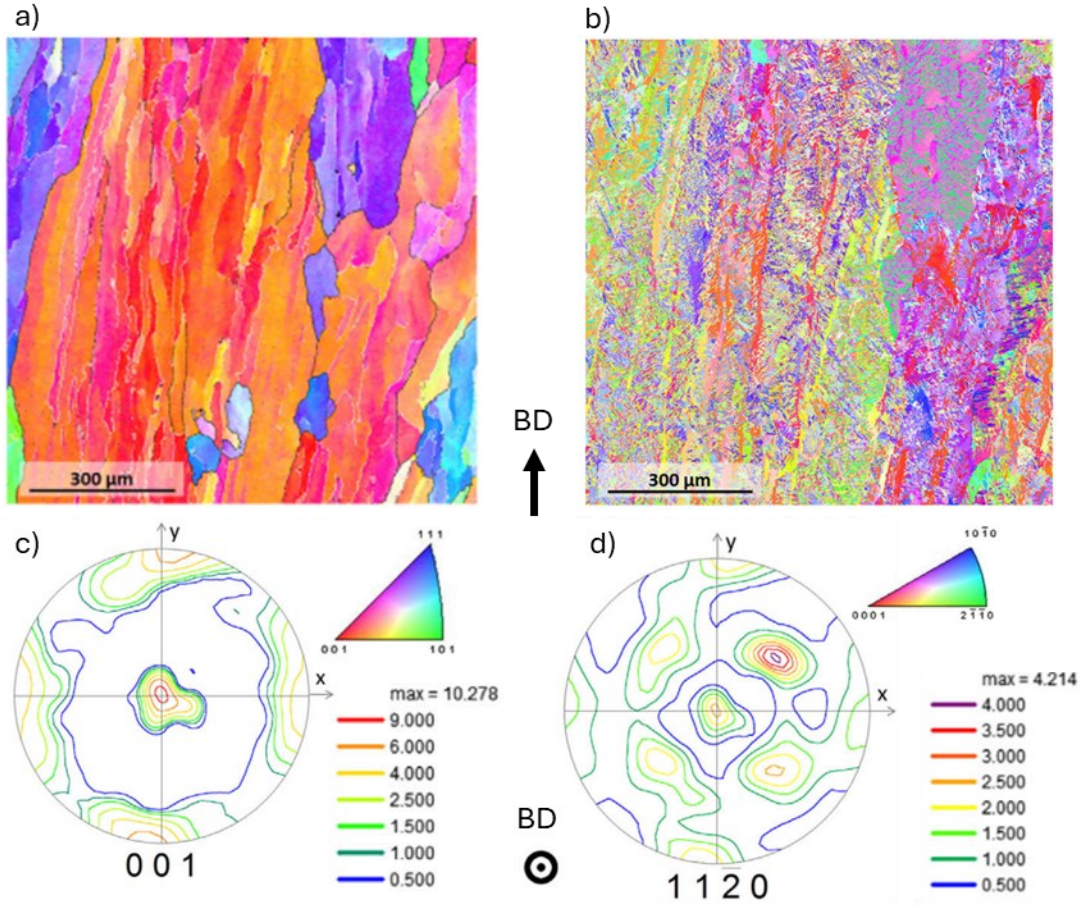


Figure 10. IPFs and PFs for the PBG reconstruction and real α/α' microstructures of as-built AM Ti-6Al-4V. **a)** and **b)** show the IPFs of the PBG and real microstructure w.r.t. the Building Direction (BD), respectively. **c)** and **d)** show the polefigures of the PBGs and final microstructure, respectively. The building direction is marked as BD, and it is the same as the z direction. PBGs have been calculated using the BOR. Adapted from ref. [38].

If the cooling rate is low enough, a lamellar $\alpha + \beta$ microstructure will form through a diffusional transformation, also known as Widmanstätten α . If cooling rate is fast, martensitic α' plates form that tend to be twinned, highly strained and contain a high dislocation density, which yields a very strong but brittle material. However, during the thermal cycling inherent to the AM process, some parts of the component may heat up enough to produce martensite decomposition, which will transform the metastable martensite into the lamellar $\alpha + \beta$. The thickness of the lamellae in lamellar $\alpha + \beta$ will also depend on the magnitude of local heating, which coarsens the microstructure, and has been shown to have an important effect on the local strength and ductility through the Hall-Petch effect [39]. Fully α' and fully lamellar ($\alpha + \beta$) microstructures can be seen

in Figure 11.a) and Figure 11.b), respectively. They can be differentiated by the appearance of twins in the martensitic laths, and the display of bright interphases between lamellae in the lamellar $\alpha + \beta$ microstructure. This bright interphase corresponds to the β phase, which forms via diffusion and is rich in V, i.e., shows brighter contrast in backscattered electron images due to larger nuclei of V.

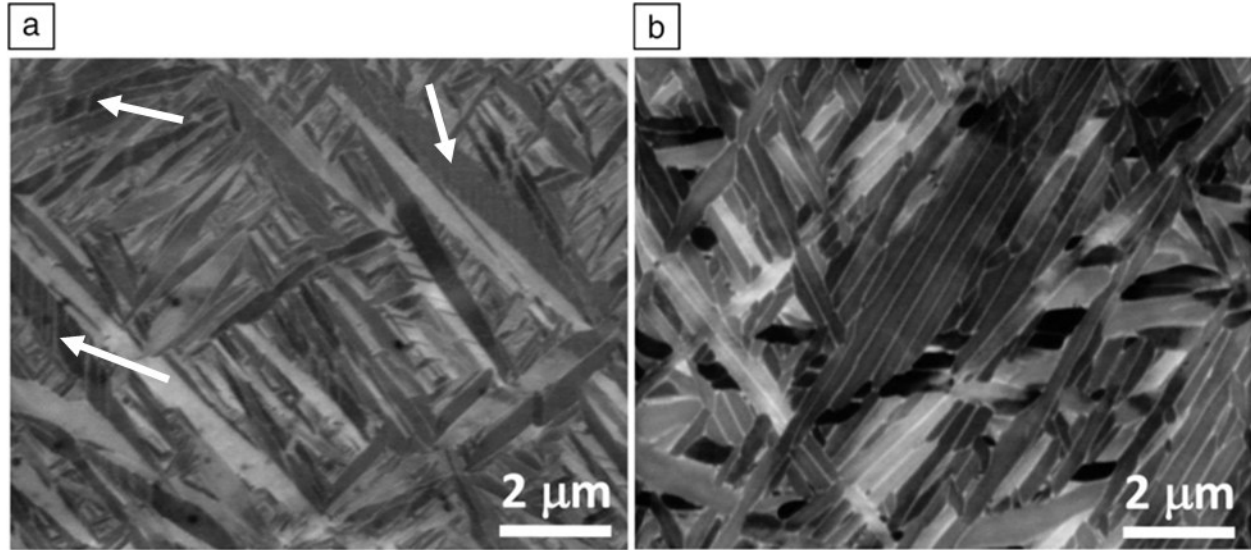


Figure 11. SEM images of Ti-6Al-4V manufactured by powder-bed fusion; **a)** fully martensitic microstructure, **b)** fully lamellar ($\alpha + \beta$) microstructure. **a)** Shows a high number of twins (highlighted with white arrows), as opposed to the lamellar $\alpha + \beta$ microstructure. β is clearly visible in **b)** at the lamellae grain boundaries due to the diffusion of V (i.e., richer in V), which makes it look brighter in the SEM image. Images extracted from [40].

Since different regions of the component experience different thermal histories, AM of Ti-6Al-4V can produce heterogeneous microstructures with changing mechanical properties along the component [8, 41, 42], as can be seen in Figure 12 from ref. [42]. This is also dependent on the key process parameters implemented during the build. Heat treatments have often been devised to homogenise and enhance the microstructure [43], and hot isostatic pressing (HIP) has been proven to remove porosity [44], but these can be expensive and time-consuming. Furthermore, heterogeneous microstructures, if predicted correctly, could be used to create tailored gradient microstructures which can be highly effective for certain desired applications [45].

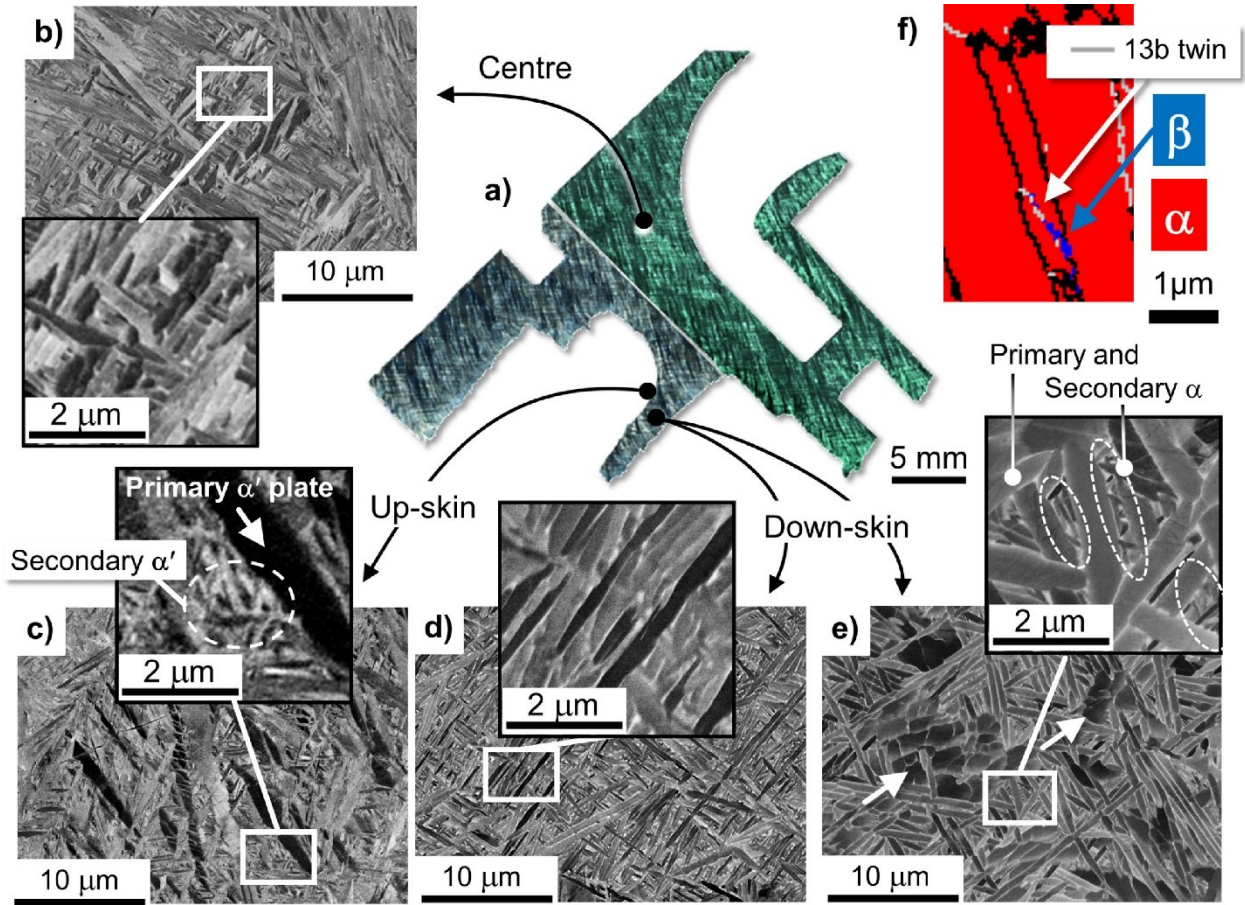


Figure 12. **a)** 2D cross-section of a laser powder bed fused impeller showing metallographic investigations along the component with Scanning Electron Microscopy (SEM), **(b-e)** lamellar $\alpha + \beta$ microstructures with varying lath thicknesses across the component, except **c)** which shows a martensitic microstructure. Figure reproduced from [42].

In summary, there is a general consensus in the literature that AM of Ti-6Al-4V produces a complex and heterogeneous microstructure whose properties are dependent on the process parameters and geometry manufactured, opening an important optimisation window in terms of manufacturing and geometrical design. As previously explained, PSPP models will be an essential tool to approach this optimisation problem.

2.3 General Approaches to AM Modelling

As previously seen, the high cost, extended build times, and numerous potential combinations of process parameters make it impractical to rely solely on experimental trial and error for defining a

metal AM process. Instead, the use of multi-physics models that can establish relationships between process parameters and the resulting material quality becomes imperative. Consequently, there has been a surge of research activity in the field of AM modelling in recent years. This section aims to provide an overview of the current state of the art in AM modelling and outline the most prevalent methods already employed in the industry together with some promising approaches being developed by academia.

2.3.1 AM Process Thermal Models

Thermal models of AM processes aim to calculate the temperature distribution throughout a 3D printed component during the printing process. Since temperature is the main driver for the development of microstructure, solidification kinetics and the generation and evolution of residual stress, understanding and reliably predicting of its magnitude and distribution is essential.

Heat Transfer Finite Element Analysis Models

Macroscopic Finite Element Analysis (FEA) models of transient (time-dependent) heat transfer allow to calculate temperature along the component throughout the whole AM process. They treat the powder and molten metal as a homogeneous continuum in a FEA simulation without resolving individual powder grains. This makes it possible to simulate the entire AM builds of relevant size and time scale. These models are already a common practice in the simulation of AM processes [46-48] and most commercial FEA codes offer workflows to perform them, usually as a first step for the calculation of residual stress. They simulate the laser as a moving volumetric heat flux. The cooling is simulated with radiation and convection to the environment together with conduction to the substrate, which is pre-heated. They also include element addition that simulates the real toolpath behaviour, which allows to account for the variation in cooling surfaces and conduction in the thermal behaviour of the process. However, it must be noted that this approach treats the powder phase and the melt pool as a homogeneous solid with different conductivities and specific heat than the solidified metal, ignoring optical and thermal interactions between powder particles and the melt pool, as well as fluid thermodynamics. This prevents this simulation from being able to account for porosity and inclusions.

Figure 13 from ref. [49] provides an example field output of these models for the simulation of the AM process of an airfoil. The results show the temperature field contour in the FEA domain at different times. Furthermore, instead of a field output contour, if the temperature during the whole process is recorded at a given node, temperature histories can also be obtained. Figure 14 shows an example of a temperature history output for an FEA simulation of a wire arc additive manufacturing process. The figure contrasts the temperature histories of two different points in different layers with experimental thermocouple measurements in the same positions. It shows how the material experiences different temperature peaks as each of the layers above the interrogated node is being printed. As higher layers get printed, these peaks attenuate as the heat is supplied at further distances from the measured node/point.

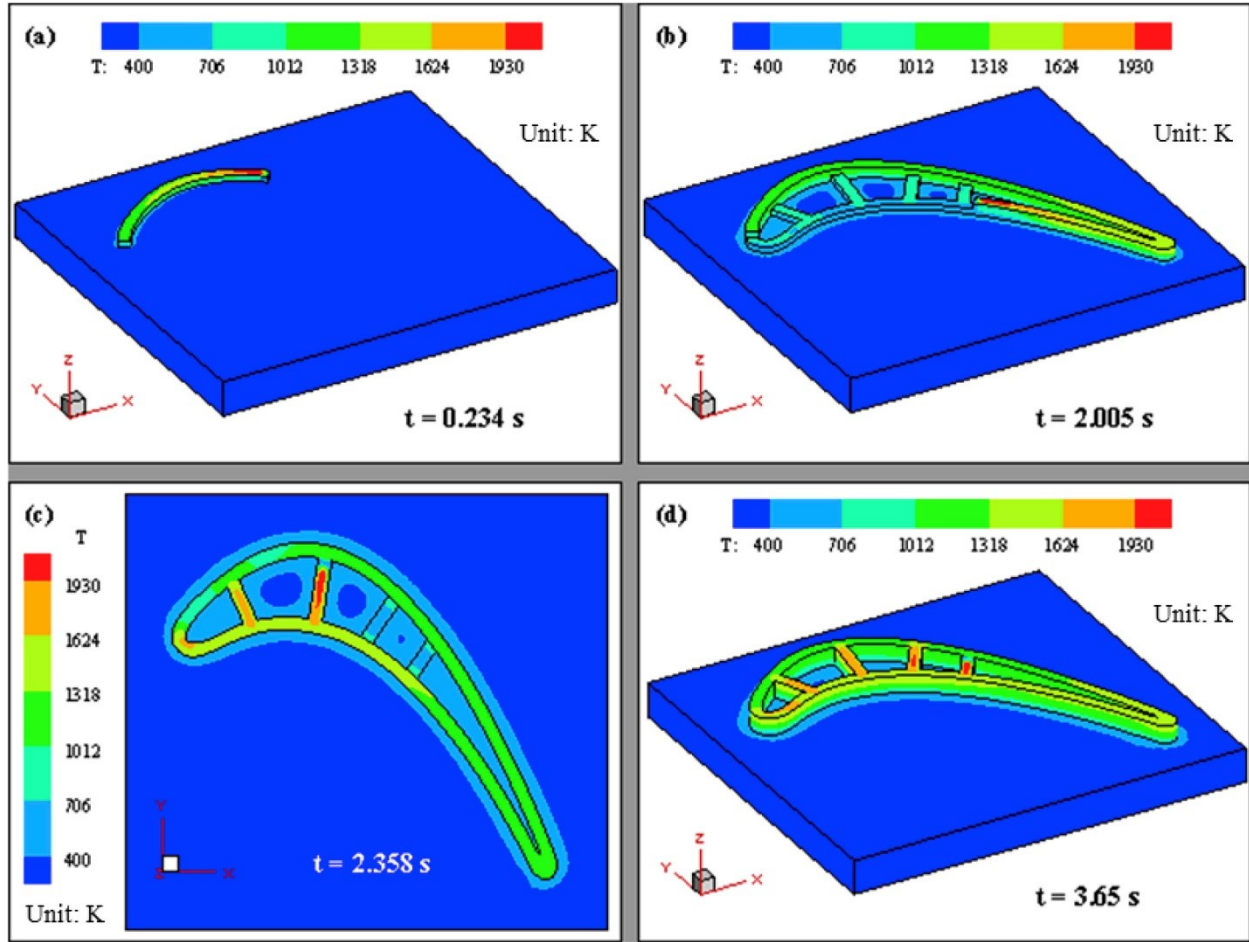


Figure 13. Temperature field output of a thermal FEA model of AM process at different times and views [49]. It corresponds to an electron beam melting process of Ti-6Al-4V, printing a complex airfoil on top of a substrate. It shows how temperature can be obtained along all the printed component at different times. **a)** $t = 0.234\text{ s}$, **b)** $t = 2.005\text{ s}$, **c)** $t = 2.358\text{ s}$ and **d)** $t = 3.65\text{ s}$.

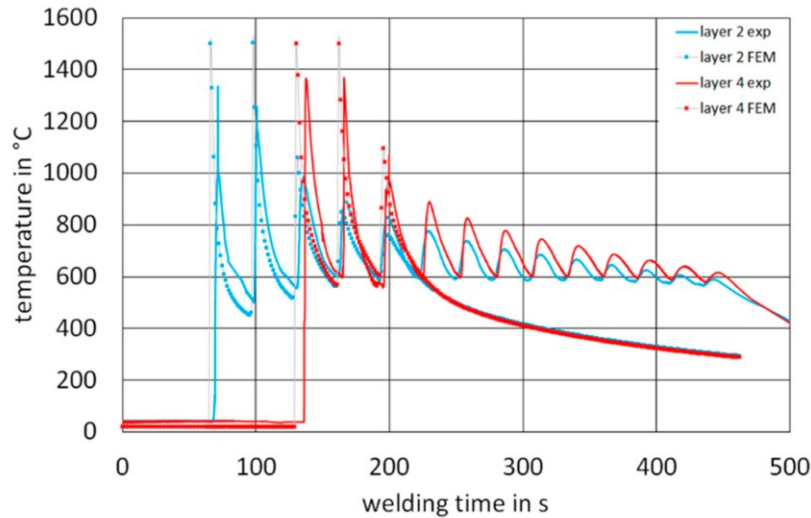


Figure 14. Comparison between temperature histories obtained from an FEA simulation and experimental thermocouple measurements. It shows the temperature histories for two different points in two different layers. It corresponds to a wire arc additive manufacturing process. Reproduced from ref. [50].

Computational Fluid Dynamics Models

Computational Fluid Dynamics (CFD) thermal models also resolve the fluid thermodynamics in the melt pool and couple it to the heat transfer calculation. Some of these models even consider the effect of different powder size distributions by considering the thermodynamic interaction of the powder particles with the laser [51]. This allows them to obtain a higher fidelity simulation which can yield more accurate thermal gradients and cooling rates in and around the melt pool and allows to predict porosity related defects like keyhole formation or lack of fusion [52, 53]. Nonetheless, these models tend to be much more computationally expensive, which makes it inadequate for them to be used for entire build simulations, whereby being restricted to only a few laser tracks. They are normally used to get an initial estimation of the expected melt pool size and its temperature field for a given set of laser parameters. This makes them very useful to get an initial optimize set of process parameters to print a given material. However, using them to obtain thermal histories of the entire AM process, which is needed to predict the microstructure of Ti-6Al-4V, is not likely to be an efficient approach. Figure 15 shows the output of a CFD-FEA model of a directed energy deposition AM process of steel 316L.

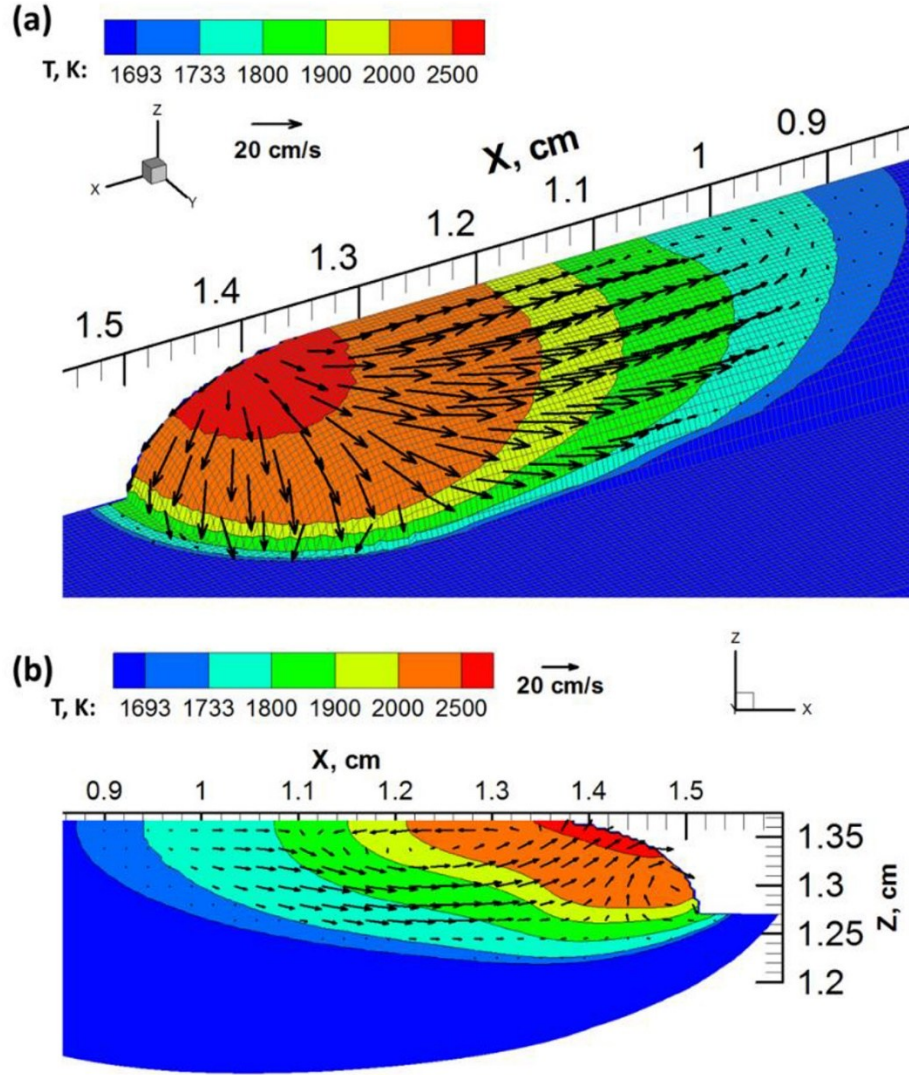


Figure 15. Temperature and velocity distributions field output of an directed energy deposition AM CFD-FEA model. It shows the curved shaped deposit for stainless steel 316L during Directed Energy Deposition. a) is a 3D isometric view and b) is the longitudinal section view, where the scanning direction is the positive x axis. Figure reproduced from ref. [54].

Analytical Models

Analytical thermal models of AM builds have been developed recently and they have the advantage of resolving the thermal history of entire builds in minutes as opposed to hours like in FEA models [55, 56].

In order to produce an analytical solution to the heat conduction partial differential equation, the non-linearity of the equations needs to be removed with certain assumptions. The main assumption is the consideration of a semi-infinite domain. This assumption is sensible in

bulk regions of components in LPBF processes, since the size of the heat source compared to the component or the substrate is significantly smaller. Another important assumption required is that the conductivity and specific heat of the material are temperature independent.

These assumptions allow to obtain an analytical equation that can be solved much faster than the FEA methods. Nonetheless, due to necessary assumptions required for solving these models, they may produce inaccurate results in certain regions like the component's boundaries, downskins or thin walls where the assumption of a semi-infinite domain does not hold well. It is also known that the temperature of the substrate during printing can change significantly, which leads to uncertainties in the implemented thermal properties which are assumed to be temperature independent.

2.3.2 Macro-scale Residual Stress Models

Controlling residual stress is a significant obstacle in the success of metal AM builds [1, 57]. Due to the localised heating of the process, metal tends to shrink during cooling after they have been printed, leading to the generation of significant residual stress fields, which can cause distortion and even cracks in cases where the stress goes beyond the material's strength [58]. The models describing and predicting residual stress aim to calculate residual stress field and the associated distortion along a component during the printing process and are mainly based on FEA, although there are some faster analytical models appearing in the literature recently [59]. Note that FEA based models of residual stress prediction follow a fairly common protocol available in most commercial FEA software like Abaqus, Ansys, Simufact and others. The two most common approaches to predict residual stress and distortions are explained in the following subsections. These are thermo-mechanical FEA models and eigenstrain FEA models. They both yield the same type of output as a structural FEA simulation, this being the residual stress tensor and displacement field (distortion) along the component. An example of the output of residual stress models can be seen in Figure 16 for the case of a thermo-mechanical FEA model, but a similar output would be yielded by eigenstrain approaches.

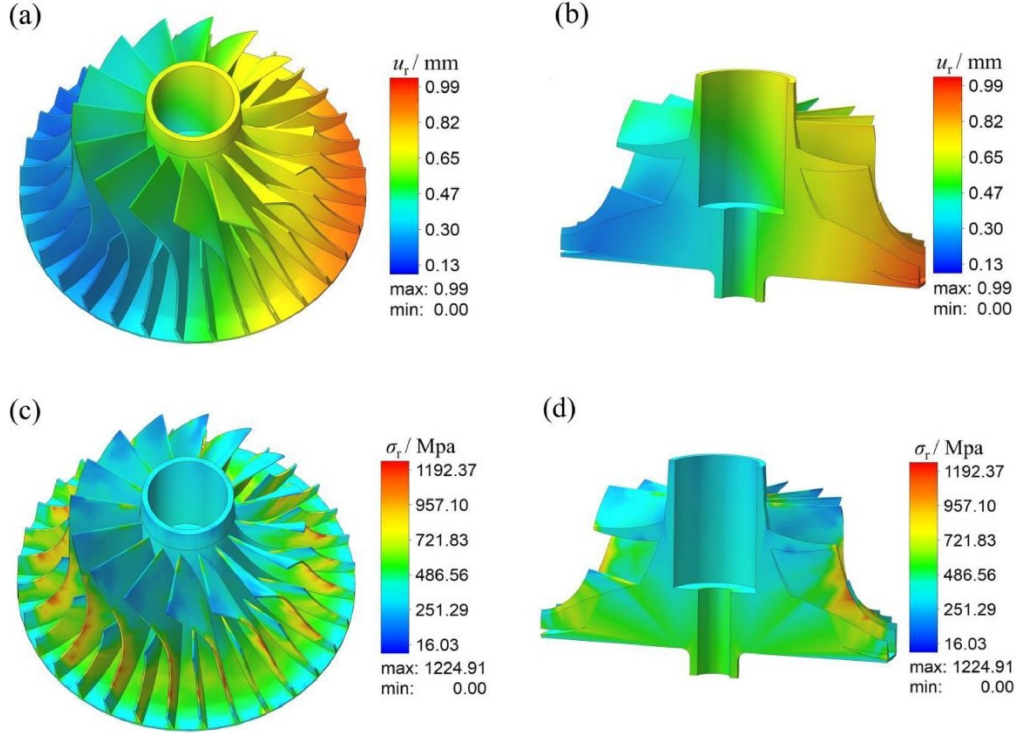


Figure 16. Example output of an FEA model of residual stress. It shows the von mises effective stress distributions and distortion field outputs of a thermo-mechanical FEA simulation of a Ti-6Al-4V impeller manufactured with LPBF; **a)** displacement contour, **b)** displacement contour view cut, **c)** von mises stress, **d)** von mises stress view cut. Images reproduced from ref. [60].

Thermo-mechanical FEA Models

Thermo-mechanical FEA models of residual stress prediction are usually solved in an uncoupled manner. Firstly, a thermal FEA heat transfer model, as explained in the previous section, is used to calculate temperature distribution along the component. This is followed by a static mechanical model, which calculates the stress field by applying a thermal expansion strain using the temperatures obtained in the previous simulation. It must be noted that these are complex models to solve and are also computationally expensive. The difficulties arise in the high non-linearities produced by the temperature dependent elasto-plastic properties required to model the process. It is also complicated to obtain these properties for less common materials [61]. Furthermore, strains produced by phase transformations are not usually predicted leading to inaccuracies in certain materials, e.g., Ti-6Al-4V [62]. Figure 16 from ref. [60] shows the output of a thermo-mechanical FEA simulation.

Eigenstrain FEA Models

Eigenstrain analysis of an AM process uses a single static mechanical step with a previously defined eigenstrain field. The elements corresponding to a given layer are added to the component at once and then its eigenstrain is introduced [63]. After the eigenstrains are applied, the residual stress field is calculated using the conventional FEA approach of static structural mechanics. Since it only requires a static step, the simulation is usually much faster than thermo-mechanical models. This approach is performed for each layer, or even a lumped sum of layers until the whole printing process is finished.

These eigen-strains represent the inelastic deformation induced by the process and therefore need to be previously known. They are usually calculated by an experimental procedure where a pre-defined small part is printed, and its distortion measured to yield the eigenstrains. Other approaches use the previously explained thermo-mechanical FEA models to calculate the eigenstrain on a small part, and the Eigenstrains obtained are used to predict residual stress in much bigger builds, saving significant computational time [64]. However, the assumption of adding entire layers at once and measuring the eigenstrain on a different geometry can lead to significant deviations and therefore worse accuracy than thermo-mechanical models.

The output of these models is a stress or displacement contour similar to the output of thermo-mechanical FEA models, which can be seen in Figure 16.

2.3.3 Microstructure Evolution Models

There are several approaches to model the chemical and morphological evolution of metallic polycrystals. Microstructure Evolution Models (MEMs) in AM use the thermal history that the material experiences during the AM process as input to estimate and predict the final microstructure. The main microstructure based models are summarised in this section, with a particular focus on the approaches that can yield a practical and reliable way of predicting microstructural characteristics, such as grain morphology, in Ti-6Al-4V components made via AM [65, 66]. These are classified into full-field and mean-field methods.

Full field methods calculate a spatial field of the microstructure usually in the form of a Representative Volume Element (RVE) containing enough microstructural features such that it

can represent the bulk material. These models contain a lot of useful data and can represent the effect of intragranular heterogeneities on microstructural evolution, but they tend to be very computationally expensive [65]. On the other hand, analytical models solve for constitutive equations usually based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model [20, 67-70] and can provide average values for phase fractions and the associated grain sizes, which can be solved almost instantly in contrast to the expensive full-field methods.

Full-Field Microstructure Evolution Models

For the sake of completeness, only Phase-Field and Cellular Automaton models are briefly described since they seem to be the ones getting the most attention for microstructure prediction in AM. However, other methods also being used include front-tracking [71], and kinetic Monte Carlo [72-74] simulations.

Phase-Field Models

Phase Field (PF) models describe microstructures as a system of continuous variables where grain boundaries have a finite width over which these variables transition between values. The evolution of microstructures is calculated based on the free energy of the system and is usually coupled to other physical properties allowing to output a complete view of microstructure character distributions. PF models of microstructure evolution normally calculate the kinetics of solute segregation throughout the microstructure and are coupled to thermodynamic databases (e.g., phase diagrams) to calculate Gibb's free energy. This allows the calculation of complex morphological features like dendrite secondary arm spacing and precipitations, which makes them the highest fidelity microstructure evolution modelling method at the meso-scale. However, these models are significantly computationally expensive due to highly coupled multi-physics involved and the need for highly refined spatial and time discretisation [75]. Due to this limitation, they are usually only used for solving a small number of grains and mostly in 2D. Furthermore, since PFM are based on minimising the free energy of the system, they are limited to equilibrium conditions, which may not always be the case in AM due to the very rapid cooling rates, especially for the martensitic transformation of Ti-6Al-4V.

Figure 17 shows the orientation and composition output of a 2D phase field simulation. The model corresponds to AM of Inconel 625 and shows a high-fidelity representation of the microstructure and its final composition with cellular growth. However, this expensive simulation is only able to represent a single track in 2D, so using this model to predict the structural performance of an entire component would be a complex task.

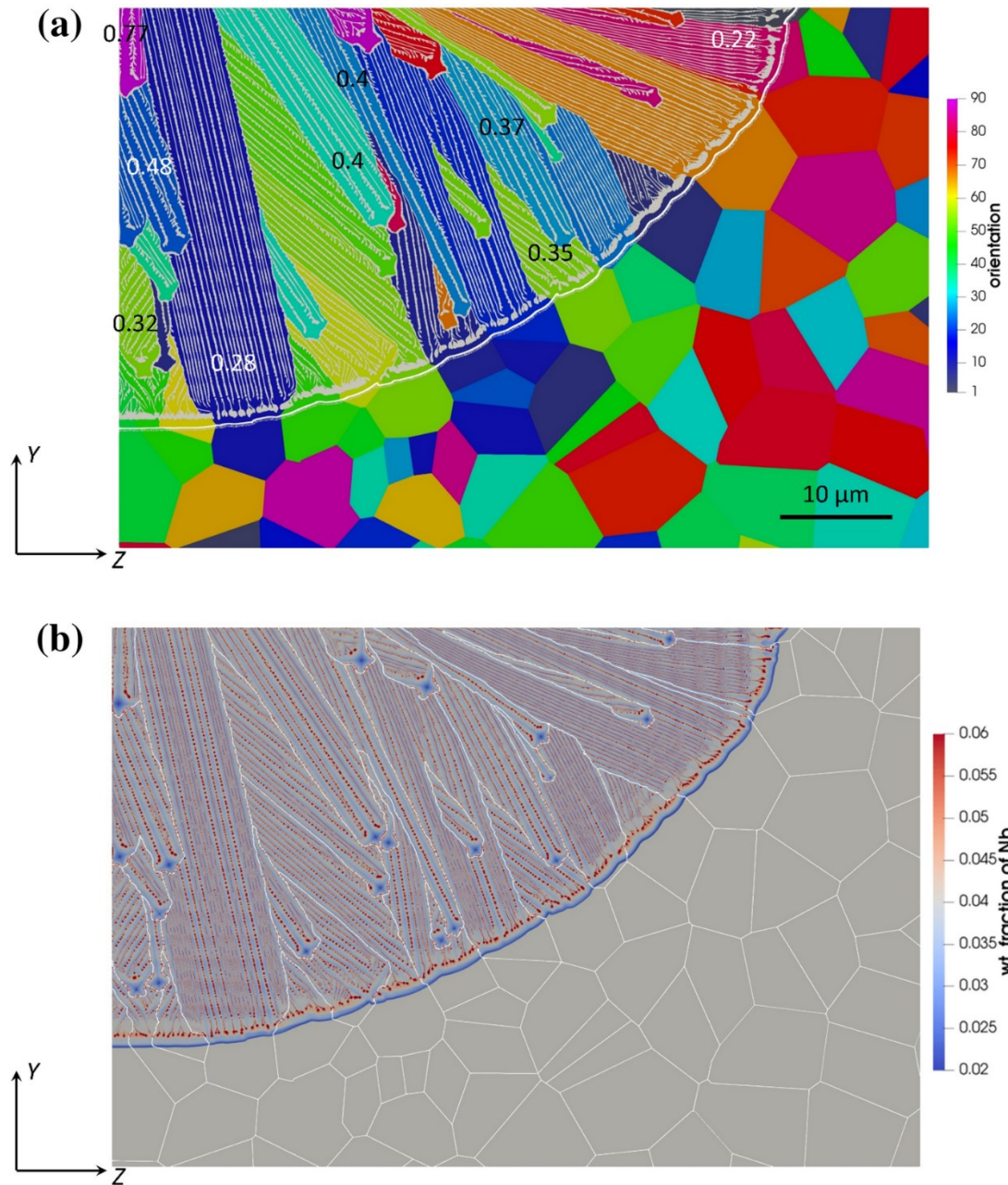


Figure 17. Output of a phase field simulation of a powder bed fusion process showing **a)** the predicted grain orientations, and **b)** solute segregation [75]. It shows the high fidelity of phase field simulations of solidification in AM, being able to resolve the cellular structure in the solidified grains.

Cellular Automaton Methods

In Cellular Automaton (CA) models, grains are represented as polyhedral building blocks and their vertices indicate the preferred crystallographic growth direction during solidification, whose growth velocities are defined by simplified models of crystal growth. The microstructure is represented in a voxelated domain where each voxel will have assigned a grain or the liquid phase [76, 77]. Then, the state of each cell will change depending on the state of neighbouring cells according to the defined crystal growth rules.

Since the state of a cell only depends on neighbouring cells, these models are much faster than PFM models, enabling them to simulate the solidification of a large number of grains or even the entire build [78], and predict the texture and grain morphology reliably with some calibration. It must be noted that in contrast to PFM, CA is not normally used to calculate any precipitation and is limited to calculate microstructure evolution only during the initial solidification. Therefore, for the case of Ti-6Al-4V, CA could only give useful information on the as-solidified PBGs, and not on the subsequent α lath microstructure. Figure 18 from ref. [79] shows the output of a CA simulation of Inconel 718 during powder bed fusion. It shows how a quite a large 3D region of the microstructure can be predicted in terms of morphology and texture.

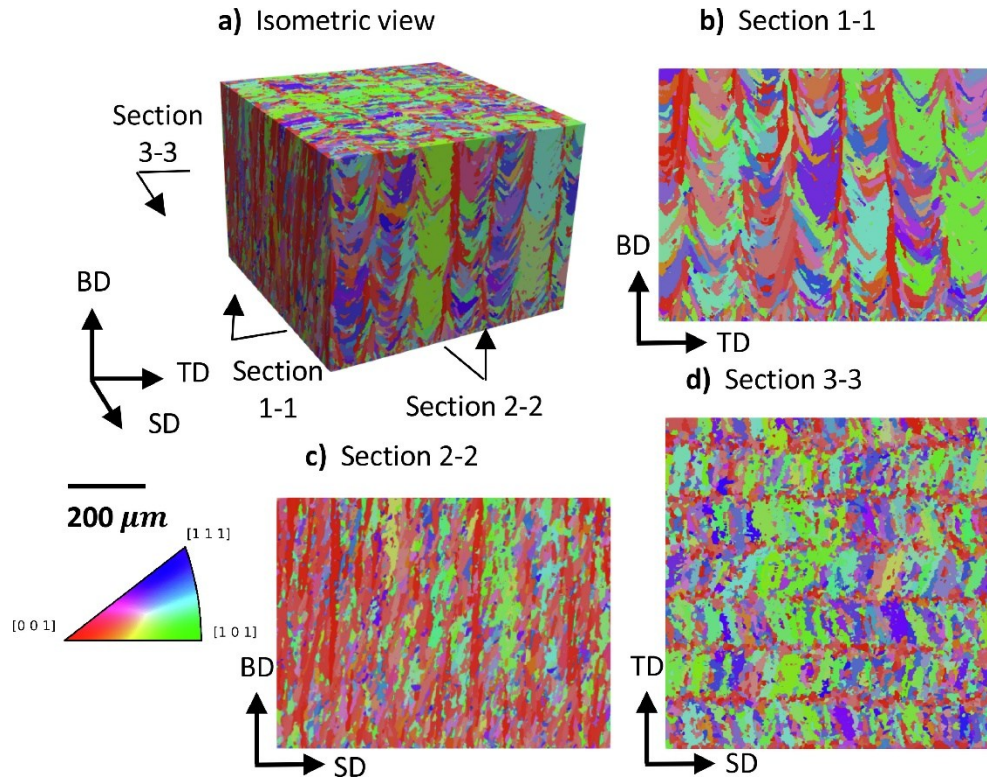


Figure 18. Output microstructure of a CA simulation of powder bed fusion of Inconel 718 [79]; it displays an IPF of the obtained microstructure with respect to (w.r.t.) the building direction from different views. It shows how CA can be used to predict large regions of solidified microstructures in terms of morphology and texture.

Mean-field Microstructure Evolution Models

Mean-field models aim to describe microstructure evolution through analytical, phenomenological equations calibrated using experimental data. Common examples include the Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation, applied to diffusional phase transformations, and the Koistinen–Marburger (KM) equation [80], used to model martensitic transformations. These models provide estimates of average phase fractions and morphological features based on the thermal or physical data of a manufacturing process.

Although mean-field approaches lack the spatial resolution and local heterogeneity representation of full-field models, they offer a major advantage in fast computational speed. By treating the microstructure in terms of average quantities rather than spatially resolved fields, mean-field models can enable rapid prediction of microstructural evolution along an entire additive manufacturing build, provided that the local thermal history is known [81-83].

Some simple example applications of mean-field models are the estimation of dynamic recrystallization in the forging of Ti-6Al-4V for different temperatures [84] or the estimation of tempering during AM of steel [85]. Both of these nucleation and growth mechanisms have been shown to be correctly estimated with the phenomenological JMAK equation, where the constant K is stated as a function of temperature, as displayed in Equation 1. Here, the constants K_0 and n are usually calculated from Time-Temperature-Transformation (TTT) or Continuous-Cooling-Transformation (CCT) diagrams from the transformation to be studied.

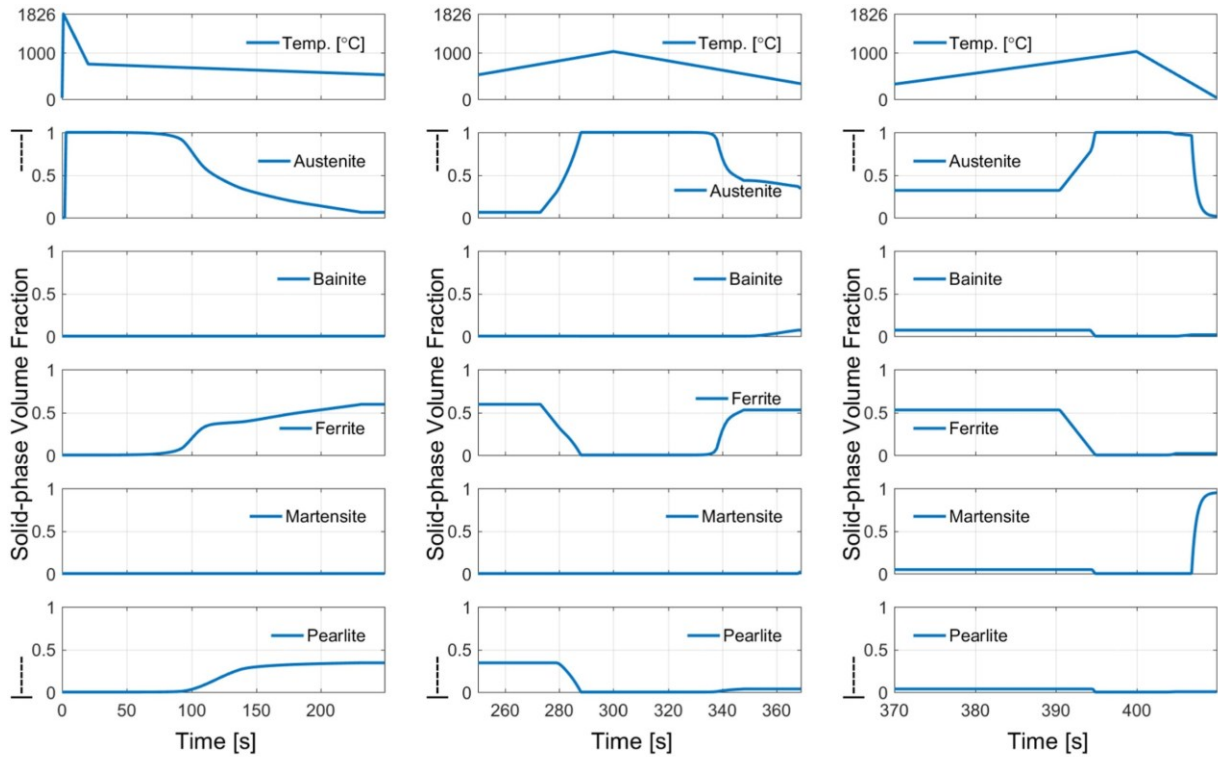
$$X(t) = 1 - \exp(-K(T)t^n) \quad \text{Equation 1 a}$$

$$K(T) = K_0 \exp\left(-\frac{Q}{RT}\right) \quad \text{Equation 1 b}$$

Beyond these phenomenological formulations, higher-fidelity mean-field models incorporate geometric information from the evolving microstructure and employ more physically based descriptions of transformation kinetics. One of the earliest examples is the Burke and Turnbull model [86], which represents the microstructure by its mean grain radius and assumes that the grain-growth rate is inversely proportional to this radius. These models provide improved accuracy in predicting curvature-driven growth and diffusion-controlled phenomena. A comprehensive overview and comparative analysis of mean-field models is available in reference [87].

An example outcome of such a model is shown in Figure 19 from ref. [81]. It illustrates the predicted evolution of average phase fractions for Steel 5140 under various thermal histories, demonstrating the capability of mean-field approaches to capture transformation kinetics across diverse processing conditions.

As can be seen in Figure 19, these models are not limited to modelling phase transformations in the literal sense, since the evolution of pearlite can also be modelled as a diffusional process with the JMAK equation. This is useful because although pearlite is not an explicit phase, but a mixture of ferrite and cementite, it is commonly treated as a single constituent unit when calculating mechanical properties.



(a) Cooling Rate = 1°C/s

(b) Cooling Rate = 10°C/s

(c) Cooling Rate = 100°C/s

Figure 19. Average phase fractions predicted by a mean-field microstructure evolution model of Steel 5140. It shows the phase fractions predicted throughout different thermal histories. Figure reproduced from ref. [81].

2.3.4 Structure-Property Models

Once the microstructure of the material is known, structure-property models aim to utilize the obtained microstructural information to calculate mechanical properties of the analysed material. They can also be classified into mean-field and full-field methods.

Mean-Field Structure-Property Models

Similar to the mean-field methods described for microstructure evolution, structure-property mean-field models calculate mechanical properties based on average values of microstructural features and phase fractions and allow for a fast calculation of mechanical properties. An example

of such a model can be found in ref. [88], which calculates the stress-strain response of Ti-6Al-4V from average values of phase fractions and morphology.

Nonetheless, one main disadvantage of these models is that they are based on experimental calibrations, which might make them inaccurate when unexpected features appear in the microstructure. Furthermore, they usually do not account for texture and are therefore not able to reliably consider anisotropic effects, which can be important in AM.

Full-Field Structure-Property Models

Full-field methods use a geometrical representation of the microstructure containing enough features such that its response to a loading state will be representative of the same loading on the bulk material. This geometrical representation is named representative volume element (RVE). RVEs can be obtained experimentally with 3D EBSDs, using full-field microstructure evolution models or with synthetic generation methods like Voronoi tessellations.

By applying a loading boundary condition on the RVE and solving the equilibrium equations using FEA or FFT methods, the mechanical strength of the microstructure can be assessed and used to derive bulk mechanical properties of the material. To solve the equilibrium equation, a constitutive model is used that is usually based on the CP model developed by Asaro and Rice [89]. CP models track the shear stress on the slip directions of the loaded crystal structure and plastically deform the material accordingly in the appropriate direction. By considering appropriate CP mechanics in an accurate RVE representation of a polycrystal, digital mechanical testing of virtual microstructures can be performed to obtain the anisotropic properties of the material such as elasticity, strength, ductility and even fatigue life [90, 91]. The input and outputs of a CPFEA simulation can be seen in Figure 20 from ref. [92]. In this figure, the microstructural RVE has been generated synthetically using a Voronoi tessellation and tested mechanically using CPFE to yield strain distribution.

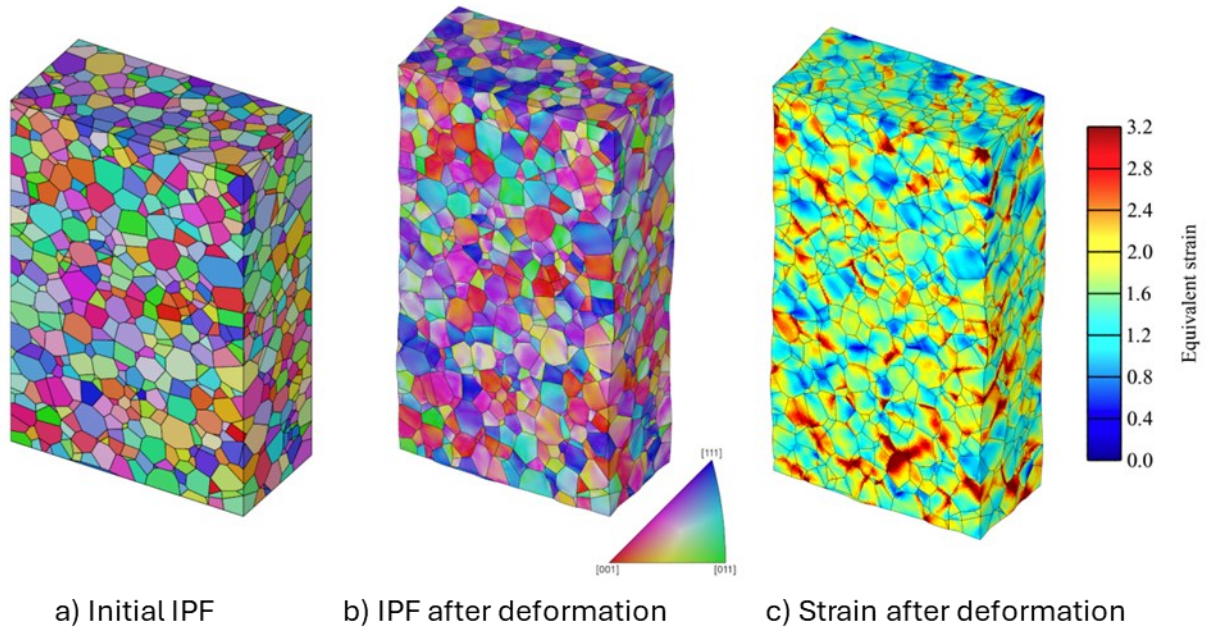


Figure 20. IPF of an RVE w.r.t. the vertical direction **a)** before, and **b)** after deformation, with **c)** showing the equivalent strain field output after deformation. It shows how CPFE can be used to analyse texture evolution and strain localisation. Figure reproduced from ref. [92].

Therefore, although computationally expensive, full-field structure-property models can intrinsically consider microstructural changes if represented in the RVE and constitutive model. These are therefore easier to apply to novel materials without requiring to re-write equations like in the case of mean-field models.

2.3.5 Process-Structure-Property Models

As previously described, process-structure-property models directly relate the process parameters used in a manufacturing process to the final mechanical properties of the manufactured component. This way, the design of a component's manufacturing and its geometry can be combined to produce the most optimal configuration for a given application. Usually, due to the different physics and scales involved, which can affect the final properties of a component during manufacturing, process-structure-property models require a combination of the several simulation models which have been described in the preceding sections.

For the case of AM, since temperature is the main driver of microstructural changes during manufacturing, as seen in Section 2.2.5; a process model that captures geometry and process

parameters and yields temperature history is used. Thereafter, the evaluated temperature history is used as input in a MEM model that is used to predict the final microstructure. The final step is a structure-property model that yields the properties associated with the local microstructure [93].

To the knowledge of the author, the only published process-structure-property models for Ti-6Al-4V available in public domain use a thermal FEA model to capture temperature and then use analytical equations both for the MEM and the structure-property model [39, 82, 88, 94]. This is probably due to the complex multi-scale microstructure evolution of Ti-6Al-4V, which is hard to predict with full-field methods. However, as explained before, analytical models do not account for texture and normally lack anisotropy considerations, and they are also difficult to adapt to morphological changes in the microstructure.

Regarding other materials, ref. [95] reported a model for Inconel 625 that uses CA for the prediction of the solidification microstructure and CPFЕ for the structure-property relations, obtaining the RVE by meshing the output of the CA simulation. The step-by-step procedure for this approach is summarised in Figure 21. A similar approach has been followed by ref. [96] for X30MnAl23-1 material, but a kinetic Monte Carlo (kMC) model was used instead for the MEM model.

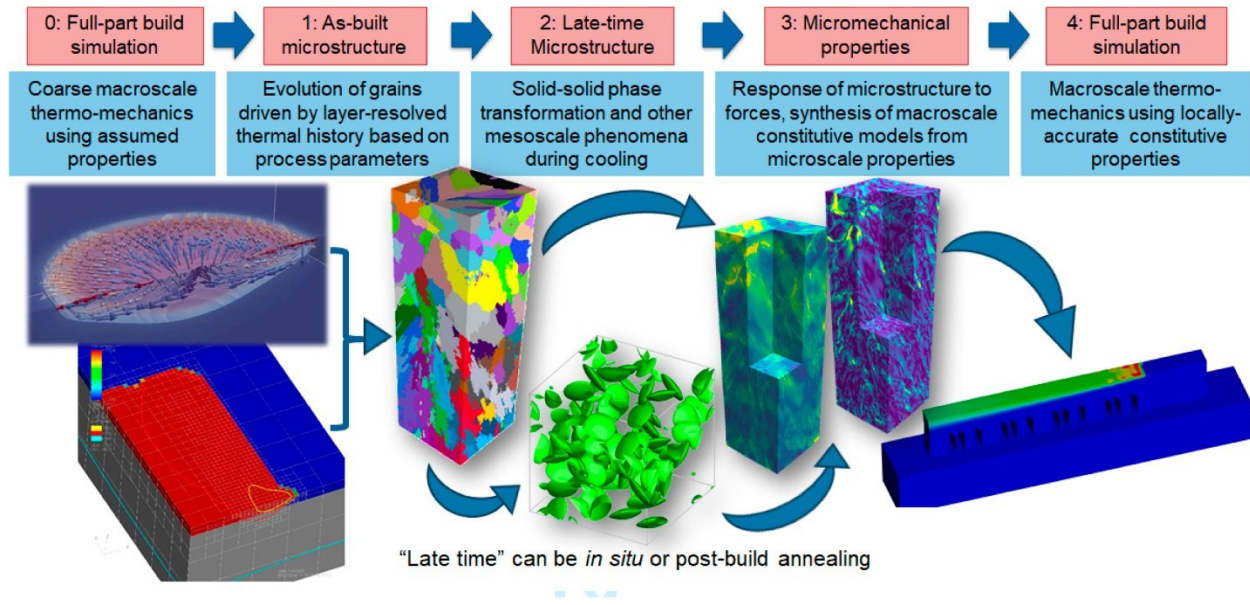


Figure 21. An overview of the process-structure-property model developed in ref. [95] for the calculation of residual stress; **0)** the approach starts with a thermomechanical macro-scale model with assumed mechanical properties, **1)** the as-solidified microstructure is calculated by combining a CFD model of the melt pool with a CA model, **2)** the late-time microstructure is calculated using a phase-field model that considers solid-state phase transformations, **3)** the mechanical properties for the obtained microstructure are calculated using a CPFE model, and **4)** the local properties are redefined, and the thermo-mechanical model is repeated. Image reproduced from ref. [95].

These approaches are highly physical and sensible and have been proven to be effective in their prediction for the studied materials. However, it would not be straightforward to use these models for Ti-6Al-4V since CA or kMC cannot predict the microstructure due to the allotropic phase changes (i.e., $\beta \rightarrow \alpha/\alpha'$) in Ti-6Al-4V on cooling below β -transus (≈ 998 °C) following solidification. In order to use these approaches, MEM models would need to account for the phase transformations of Ti-6Al-4V. Although there exist some phase-field models for $\beta \rightarrow \alpha$ transformation [97-99], they can only be implemented to scales much smaller than a typical parent β grain size (i.e., usually in mm) and it is unclear if they are able to simulate all types of solid-state phase transformations in Ti-6Al-4V during the thermal cycling of an AM processes, especially the displacive martensitic transformation as the yielded α' grains are significantly smaller.

2.4 Justification of chosen Process-Structure-Property-Performance modelling approach

The presented literature review showed that, to the knowledge of the author, current public-domain PSPP models for AM of Ti-6Al-4V are limited and resort to simplified analytical equations for the calculation of elasto-plastic properties, which fail to capture critical effects such as crystallographic texture and anisotropy. This lack of models is attributed, on one hand, to the solid-state transformations that occur in the already solidified material during the process, which require to evaluate the entire thermal history and not only the solidification process. On the other hand, the yielded heterogeneous microstructure is intricate to model due to its complex geometry and anisotropy. This presents a clear knowledge gap that the proposed PSPP model in this work aims to resolve. The following subsection explains and justifies the approach of the developed PSPP model in this work and how it resolves this knowledge gap.

As has been discussed, most current Process-Structure-Property AM models start with a simulation of the manufacturing process that can quantify the thermal histories experienced by the material, followed by a full-field microstructure evolution model, such as CA, which predicts the final microstructure, and finally a structure-property model based on CP that can yield the microstructure's mechanical properties. These already developed process-structure-property models happen to study materials whose microstructures are solely defined during the initial solidification, which makes the models simpler since a MEM model of solidification and a process model that only considers the initial melting suffices to yield the final microstructure. For the case of Ti-6Al-4V, the mechanical properties are mostly dependent on solid state phase transformations which occur on cooling significantly below the solidification temperature (between β -transus and M_f), since most β transforms to α or α' . In practice, the initial as-solidified microstructure does not need much attention since, due to the epitaxial growth of Ti-6Al-4V in LPBF, it ends up being a consistent and homogeneous microstructure of columnar prior β grains with low dependency on process parameters [100]. For these reasons, process-structure models of Ti-6Al-4V must account not only for the initial melting and solidification stages but also for the subsequent temperature evolution and phase transformations that occur throughout the entire additive manufacturing process, i.e., during the printing of all above layers.

Therefore, regarding the thermal process model, a transient heat transfer FEA model seems like an adequate choice. A CFD model would not work since it would be computationally impossible to simulate large builds and the cooling rates and thermal gradients around the melt pool do not influence Ti-6Al-4V microstructure significantly. Analytical models based on the

Rosenthal equation [55, 56] could be used, but they could not guarantee accuracy in many regions like downskins and other surfaces due to their assumptions, which tend to be structurally critical.

For the MEM models, analytical models seem to be the only option for Ti-6Al-4V due to the intricate physics regarding its solid-state phase transformations. Although phase field models could theoretically simulate them, they remain very computationally expensive, and there are not existing models for martensite decomposition, which is an essential phenomenon to consider in estimating the mechanical properties of AM Ti-6Al-4V. Therefore, an analytical model has been chosen instead since it can yield the final microstructure rapidly and they are already quite developed for the phase transformation of Ti-6Al-4V during AM, despite not being as predictive in terms of microstructural morphology.

Next, for process-structure models, CP models based on RVEs seem to be the most practical option since they can intrinsically consider the effect of different textures, phase fractions and grain sizes on the anisotropic tensile properties of a given microstructure. Although analytical structure-property models exist for Ti-6Al-4V, these need extensive experimental calibration and significant material science knowledge if they need to be modified for novel alloy compositions or AM processes. If a CP model is to be used from analytical model results, the RVE will need to be generated synthetically using a geometrical method like Voronoi tessellations.

Finally, the local mechanical properties computed are introduced into a structural FEA model in order to assess the structural performance of the simulated component against arbitrary design loads.

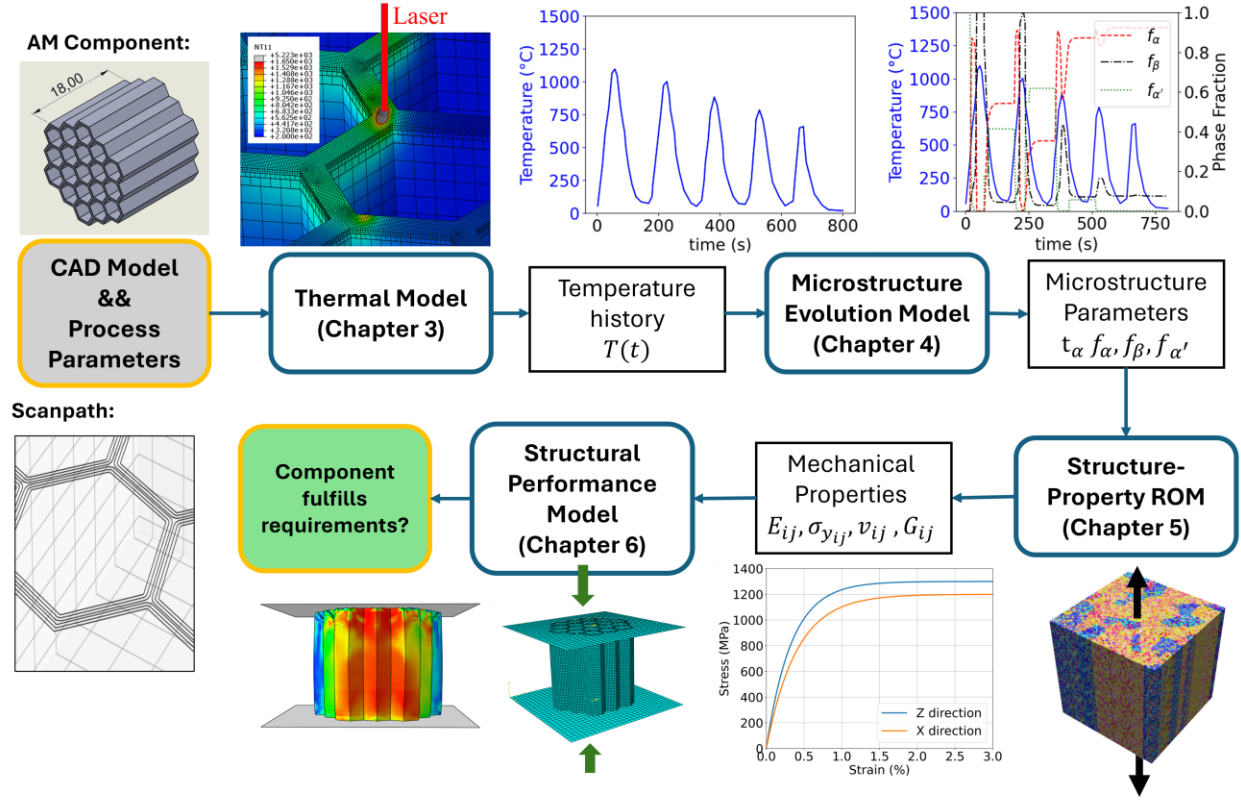


Figure 22. Schematic representation of the developed PSPP framework in the presented work, showing an example for a 3D printed honeycomb. It illustrates how the chapters of the thesis are organized around the independent models that constitute the PSPP chain. The diagram shows how a structural FEA model with spatially resolved mechanical properties is generated from the input CAD geometry and process parameters. This is achieved through a thermal FEA model that provides local temperature histories, a microstructure evolution model that predicts the resulting local microstructure, and a crystal plasticity Reduced Order Model (ROM) that determines the corresponding local mechanical properties. Reproduced from Figure 2.

In summary, based on the insights obtained from the literature review and the considerations outlined above, the following methodology for PSPP modelling of Ti-6Al-4V was adopted. Firstly, a thermal FEA model is used to calculate the full temperature history of the AM process. Then, it is followed an analytical MEM that uses this temperature history and computes the key microstructural information that drives mechanical behaviour. Next, this is coupled with a synthetic RVE generation and a CP model that relates microstructure to properties. Finally, the local mechanical properties computed are input into a structural FEA model for performance analysis against an arbitrary load. This novel approach allows to calculate the full thermal history and model the solid-state transformations that occur during the entire process, while also

considering their effect on elasto-plastic mechanical properties and anisotropy. To the knowledge of the author, a PSPP approach like this has never been presented and could have important benefits for the optimization of AM processes.

This developed PSPP model in this thesis is illustrated in Figure 22. As each model can be used independently, they are presented along the thesis in distinct chapters, where their respective modelling methodologies are described and the developed models are analysed with experimental validation. The thermal model is explained in **Chapter 3 - Thermal FEA Model of LPBF for the prediction of Phase Transformations**, the microstructure evolution model in **Chapter 4 - Microstructure Evolution Model of Ti-6Al-4V**, the structure-property model in **Chapter 5 - Microstructure-Property Modelling of Additively Manufactured Ti-6Al-4V**, and lastly the structural performance model with local mechanical properties in **Chapter 6 - Process-Structure-Property-Performance Modelling of Additively Manufactured Ti-6Al-4V**.

3. THERMAL FEA MODEL OF LPBF FOR THE PREDICTION OF PHASE TRANSFORMATIONS

As explained in the literature review (Chapter 2), the local microstructural features in a Ti-6Al-4V part built by AM depend mainly on the local thermal histories that a given point experiences during the AM process. Therefore, the first step in creating a PSPP model framework for this material is to predict these thermal histories accurately throughout the whole process. To do so, a thermal FEA model seems appropriate since it is reliable to calculate thermal evolution at the range of temperatures where the solid-state phase transformations of Ti-6Al-4V occur. This chapter explains the modelling methodology and the experimental proof of a thermal FEA model of LPBF for the purpose of predicting microstructural evolution during this process.

Macro-scale thermal FEA models are already a common practice in the simulation of AM processes [46-48]. The schematic of the AM macro-scale thermal FEA model developed in this work is displayed in Figure 26, for which detailed information can be found in the methodology section (Section 3.1). It must be noted that this approach treats the powder phase and the melt pool as a homogeneous solid with different conductivities and specific heat than the solidified metal, ignoring optical and dynamic interactions between powder particles and the melt pool, as well as fluid flow and thermodynamics. As a result, this approach does not permit the simulation to account for porosity defects, which have been neglected in this work. Nonetheless, the manufacturing approaches to minimise these defects are mostly well known and documented [101], so in this work the focus is on how to estimate the mechanical properties assuming a fully-dense component.

This type of macro-scale FEA thermal simulations are usually performed for its use in a sub-sequent structural simulation for the prediction of thermal stress distribution and the associated distortion [102]. These structural simulations use the calculated thermal histories as input to apply thermal expansion strains. They yield an estimate of the residual stress and distortion in a manufactured component. It must be noted that the work presented is not a substitute for this simulation approach. However, instead on focusing on residual stress and distortion prediction, the aim is to predict microstructure characteristics in the component which can then be used for the prediction of local mechanical properties. Note that both approaches can be used together to assess the mechanical response and properties of a component. In fact, the results from the MEM could

be used in the structural simulation to apply phase transformation strain [103], and the results from the CPFE simulation could be used to estimate the mechanical properties, increasing physical fidelity of the results in predicting residual stress.

3.1 Modelling methodology

The transient thermal FEA model used in Abaqus Standard solves the non-uniform isotropic heat conduction PDE, displayed in Equation 2 a, where T is the temperature, H is the enthalpy, t is time, c_p is the specific heat, k is the conductivity and ρ is the density. To accurately model transient heat transfer with temperature-dependent material properties, which make the problem non-linear, the governing equations are formulated in terms of volumetric enthalpy to ensure strict energy conservation. Numerically, Abaqus resolves this non-linear system using an implicit backward-difference time integration scheme paired with an iterative solver. Within each discrete time increment, the solver estimates the new nodal temperatures, evaluates the temperature-dependent properties (k, ρ, c_p) from user-provided tabular data to integrate the total internal energy state, and iterates until the residual error of the global energy balance converges to zero.

$$\frac{\partial H}{\partial t} - \nabla \cdot (k(T) \nabla T) = Q(x, y, z, t) \quad \text{Equation 2 a}$$

$$dH = \rho(T) c_p(T) dT \quad \text{Equation 2 b}$$

The right-hand side of Equation 2 a, $Q(x, y, z, t)$, includes the heat sources and losses in the FEA domain. For a LPBF model, these are the heating from the laser beam and cooling due to convection and radiation. Laser heat is modelled as a moving volumetric heat flux using Goldak's semi-ellipsoid model [104] in Equation 3, which is shown schematically in Figure 23. Each node inside the defined ellipsoid experiences heat flux according to this equation, and the local reference frame used displaces in time according to a specified toolpath.

$$Q_{laser} = \begin{cases} q_f & \text{when } x \geq 0 \\ q_r & \text{when } x < 0 \end{cases} \quad \text{Equation 3 a}$$

$$q_{f/r}(x, y, z) = \frac{2P\alpha}{abc_{f/r} \pi \sqrt{\pi}} \exp \left[- \left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c_{f/r}^2} \right) \right] \quad \text{Equation 3 b}$$

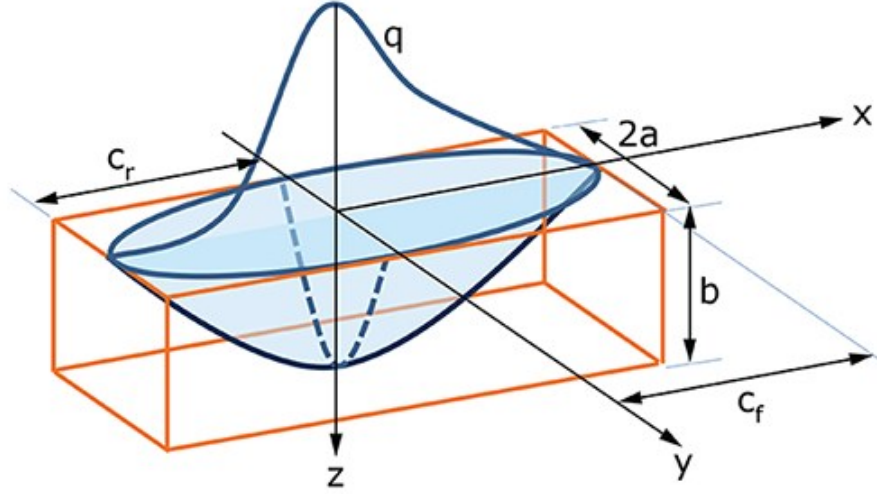


Figure 23. Goldak's semi-ellipsoid expression for laser heat spatial distribution [105] used in the FEA model to consider laser heat. The laser scanning direction is the positive x axis. The parameters are explained in Equation 3.

In Equation 3, α is the absorptivity coefficient and can be measured experimentally [106], usually assumed constant in numerical models. Goldak's geometrical parameters can be approximated to be related to the laser parameters of a LPBF build as $a = er$, $b = r/e$ and $c = d$, where e is the eccentricity, d is the penetration depth and r is the laser spot radius at the surface of the powder layer. For most LPBF systems, e can be approximated to be equal to 1 and the penetration depth d can be approximated to the thickness of a layer [81]. The laser spot radius r depends on the Focal Offset Distance (FOD). The effect of the FOD on the laser spot radius at the surface can be seen in Figure 24. The radius at the surface r can be calculated using Equation 4 [107], where r_0 is the laser radius at focus and Z_r is the Rayleigh length of the laser system. The Rayleigh length Z_r is the FOD at which the laser beam's cross-sectional area doubles. Both Z_r and r_0 are constants for a given laser system and can be measured, and the FOD is usually a process parameter that can be chosen during an AM build.

$$r(FOD) = r_0 \sqrt{1 + \left(\frac{FOD}{Z_r}\right)^2} \quad \text{Equation 4}$$

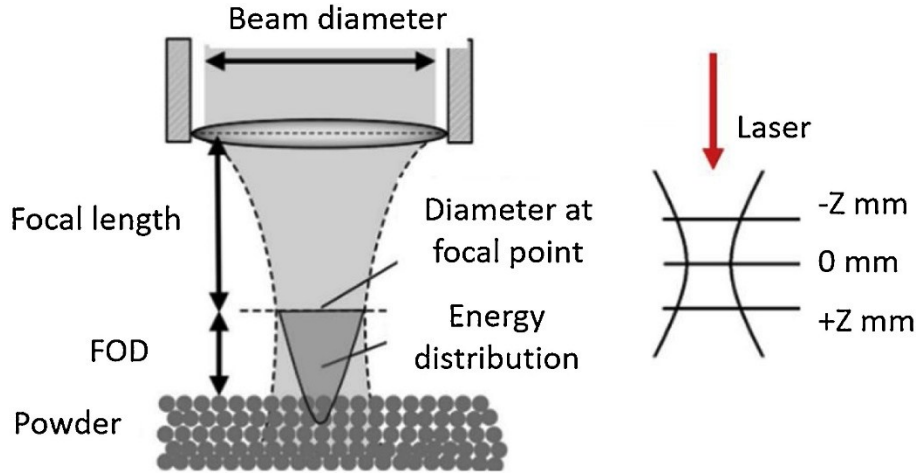


Figure 24. Schematic of the effect of changing the Focal Offset Distance (FOD) in a LPBF process. It shows changing the FOD changes the area of interaction between the laser beam and the powder. At the focal point, the area of interaction is at its minimum. Figure reproduced from ref. [107].

The cooling is simulated with volumetric thermal radiation $q_{rad} = \epsilon\sigma((T - T_z)^4 - (T_{amb} - T_z)^4)$ and surface convection to the environment $q_{conv} = h(T - T_{amb})$. Usually, LPBF machines allow to set a Build Plate (BP) temperature during the build, which is achieved and maintained with electrical heating. To model this, a fixed temperature boundary condition at the bottom surface of the build plate is applied, which is a common approach [81].

To model material addition, element addition to the FEA domain during the analysis is considered. This element addition simulates the real toolpath behaviour, in which elements are added at the same speed as the recoater movement. This accounts for the variation in cooling surfaces and conduction in the thermodynamics of the process as material is added, as well as the cooling effect of adding powder on top of the hot printed material.

To consider the transient interaction of the moving toolpaths corresponding to the material addition and the moving heat source with the FEA domain, Abaqus offers a toolpath-mesh intersection module [105]. This module automatically calculates the elements of interaction with the laser or recoater based on an input toolpath in the form of tabular data. To generate this data, the scanpath produced by the CAM software of the AM machine has been translated into the

desired format using the Python library libSLM [108]. This library yields the vector path of the laser, and knowing the laser scanning and jump speed, the exact position of the laser could be determined at all times through kinematics. This was expressed in tabular data for every layer to be read by the toolpath-mesh intersection module.

Regarding meshing and time increments; to reduce computational cost, thermal AM simulations that are implemented in most commercial FEA software like Simufact Additive or PanOptimization for the purpose of residual stress predictions tend to use a lumped sum approach in their FEA discretisation. This consists of having a mesh element size that contains several layers along its height, called a lumped sum. Each lumped sum of layers is added at once together with its heat input by applying a large time increment. A schematic of the lumped sum method can be seen in Figure 25.a). This approach is accurate enough to get the temperature history needed for residual stress predictions. However, when predicting phase transformations, this approach cannot be used and the process has to be modelled at the melt pool scale. This is because some of the phase transformations happen in time scales much smaller than the time it takes to print an entire layer. Therefore, calculating them requires a much finer discretisation in terms of mesh size and time increments, as shown in Figure 25.b). Figure 25 shows the difference between thermal FEA models using the lumped sum approach and those that simulate the melt pool. The latter requires a much finer mesh and smaller time increments.

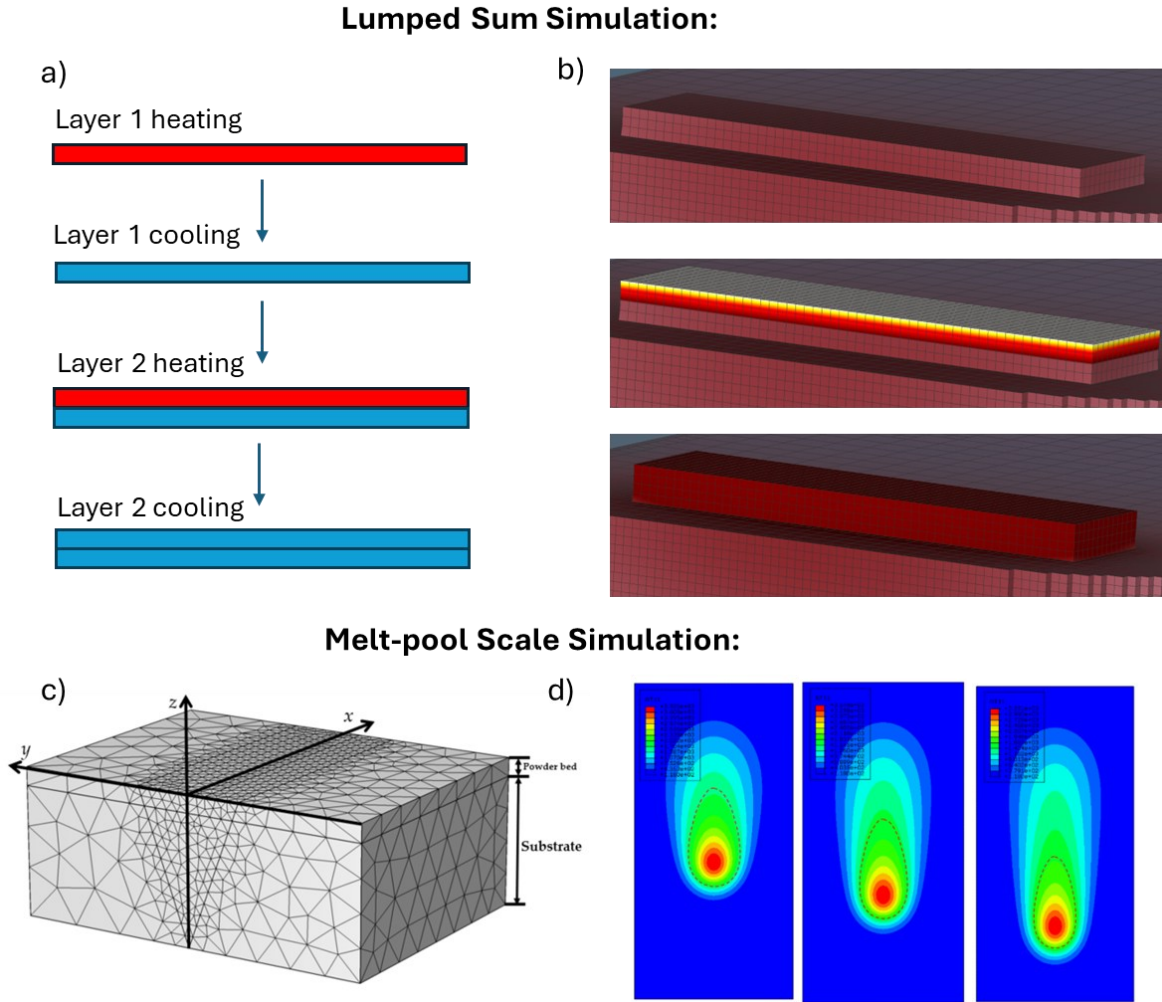


Figure 25. Differences between lumped sum and melt pool scale approaches to thermal FEA modelling of AM. **a)** Schematic of lumped sum approaches that add entire layers and their heat inputs at once. This approach is usually used for thermo-mechanical FEA modelling of residual stress. **b)** Temperature output and the mesh used at 3 consecutive time increments in the lumped sum approach from Simufact Additive [109]. **c)** Mesh size for a melt-pool scale simulation. **d)** Temperature contour output at 3 consecutive time increments in the melt-pool scale approach [110].

In this work, the developed thermal FEA model consists of a combination between these two approaches, accomplished through adaptive meshing and adaptive time incrementation. These were needed as AM simulations can be prohibitively expensive if the discretisation is not approached correctly. The time and spatial discretisation used are explained in detail in the following sections together with the temperature dependent material parameters chosen. This approach yielded an efficient method to calculate the thermal histories with the resolution needed to calculate phase transformations in AM of Ti-6Al-4V. The software framework developed for

this model has been implemented as a Python library, with a link to the corresponding repository provided in Appendix A.1. A schematic of the model developed together with example field and history outputs can be seen in Figure 26.

Figure 26.d) shows an example of a temperature history yielded by the model at a given point. It starts with a high peak when the point melts and solidifies as it is scanned by the laser. This is then followed by smaller peaks while the layers above are scanned, which produces a heat wave for each layer. These peaks get continuously smaller as the laser scans layers that are more distant (i.e. higher layers). The plot also shows that the material experiences residual heating as more layers get printed. Once the printing is finished, at around $t \approx 80$ s, the material starts to cool down as no more heat is supplied.

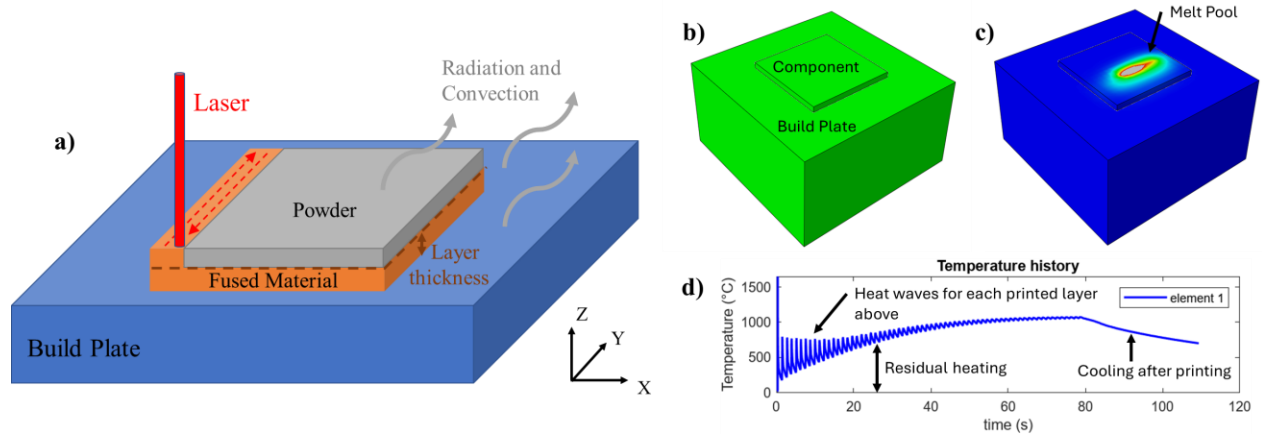


Figure 26. **a)** Schematic of the developed FEA thermal model showing the scanning of the second layer over an already fused layer. **b)** Assembly used in Abaqus showing both the build plate and the component to be printed. **c)** Example field output temperature contour, where the melt pool is shown in grey by applying this colour to all temperatures above T_{melt} . **d)** Example of temperature history output. It shows the temperature at a given node of the component throughout the whole process.

3.1.1 Adaptive Meshing Strategy

Since the melt pool in LPBF is around 50-200 μm in diameter, melt pool scale simulations, required for the prediction of phase transformation, need a small element size in the proximity of the heat source. This is caused by the high thermal gradients in this area, which require many elements to be computed correctly. Inversely, regions far from the melt pool have significantly lower gradients and can have a much coarser mesh. Adaptive mesh refinement techniques, where

the mesh is automatically refined around areas with high thermal gradients and coarsened around those with low gradients, can be very efficient for AM simulations [111, 112].

For this work, a layer-wise adaptive mesh refinement approach has been developed. This technique consists of changing the mesh every time a new layer is added, coarsening the layers far from the current layer being printed, where the thermal gradients are lower.

To allow for steep transitions of element size, tie constraints have been applied, which enable the use of a discontinuous mesh with hanging nodes. Hanging nodes are the nodes which are not connected to different nodes in adjacent elements (i.e., connected to a face or edge of an adjacent element). To ensure a continuous FE solution at these nodes, additional constraints are added on the values of the solution at these nodes, which yields additional equations to be solved in the FE computation. This can increase the computational cost of the simulation, but in FE solutions with large and localized gradients, a steep transition in mesh size using hanging nodes can produce a much more efficient computation [113].

In this modelling approach, the different element sizes for all the different layers were automatically generated from a CAD model of the component. For each layer, the mesh was generated by performing the necessary slices on the component and substrate. The top slice had a thickness equal to the layer thickness of the AM process, and the thickness of each subsequent slice was doubled. Then, different element sizes were applied to each slice. For the simulations in this thesis, an element size with an edge length equal to the layer thickness has been used for the top 3 layers, which surround the melt pool. This element size around the melt pool was shown to be accurate in ref. [81] to predict microstructure evolution in PBF of Ti-6Al-4V, although the required mesh size is likely dependent on printing parameters as well. A mesh size sensitivity has been carried out in Appendix C. Then, the characteristic element size was doubled for each slice below. Finally, the different slices were joined by a tie constraint. The meshing strategy can be seen in Figure 27. Linear hexahedral elements were used for all the thermal simulations in this thesis.

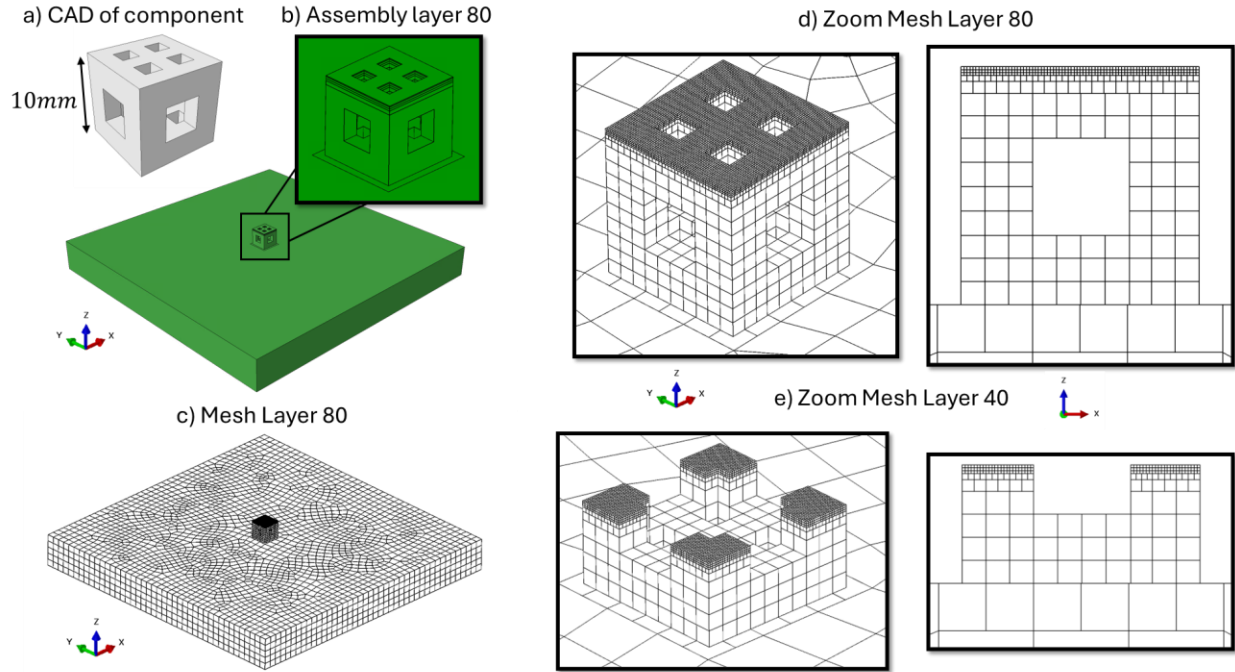


Figure 27. Adaptive Meshing strategy. **a)** CAD model of an example component to be printed, which consists of a 10 mm cube with square holes for this demonstration. **b)** Abaqus assembly at a given layer showing how the component and the build plate has been cut into slices that allow to produce different mesh sizes in different regions. These different slices are then joined by tie constraints. **c)** The mesh used at layer 80, **d)** and **e)** show isometric and view cuts of the mesh for two different layers around the component. The finest elements, which are in the top layers, have a side length of 0.6 mm, which corresponds to the layer thickness used in the printing process.

Every time the mesh is refined during a transient simulation, the current results are mapped from the current elements to the new refined mesh. This has been performed in this work using the existing mesh-to-mesh solution mapping tool in Abaqus. This tool linearly interpolates the nodal output from a different mesh to the current mesh before an Abaqus job is started. In this case, it is used to interpolate the temperature output in the simulation of a specific layer to the new mesh for the next layer. Therefore, Abaqus requires each layer to be simulated in a different job and its own output file. The mesh generation, job management and output integration to calculate the temperature history throughout the whole process were automated using an in-house developed framework in Python.

It must be noted that adaptive mesh refinement techniques for AM FE simulations are an active area of research, and more efficient techniques have recently been reported using open-source FEA libraries [114]. However, to the knowledge of the author, this is the first adaptive mesh refinement framework developed for AM in a reliable commercial FEA package such as Abaqus.

3.1.2 Adaptive Time Increment Strategy

Despite using the adaptive meshing strategy, the simulation remains computationally expensive, and it is not feasible to resolve the melt pool along the entire component with small time increments. Instead, the developed model implements an adaptive time incrementation strategy, resolving the melt pool only around a few selected points of interest where the temperature histories will be computed. Around these points, the applied time stepping is kept low enough to resolve the melt pool, and therefore obtain a reasonably accurate temperature histories required for the prediction of phase transformations. For the rest of the component, much higher time increments are applied since the temperature histories are not calculated elsewhere. This approach speeds up the simulation significantly.

To accomplish this, an imaginary sphere is positioned around each of these selected points of interest. Every time the laser path enters a sphere, the time increment is reduced to 1 ms , which has been shown to be small enough to predict phase transformations in Ti-6Al-4V [81]. When the laser moves outside of the spheres of interest, the time increment is increased to 60 ms to reduce the computational cost. The times of intersection with the spheres are calculated before the inception of the simulation for each layer, using kinematic equations with the known scanpath. Then, using the Abaqus *TIME MARKS keyword, the time increments are set to the desired values between the obtained intersection times. The implemented adaptive time increment strategy is visualised using field outputs in Figure 28. An analysis on the effect of this adaptive time incrementation strategy on the computed temperature histories has been performed and is described in Appendix B. The analysis shows that using a sphere with radius of 0.3 mm yields similar results to using a constant time increment of 1 ms , reducing the runtime of the simulation significantly while providing similar accuracy.

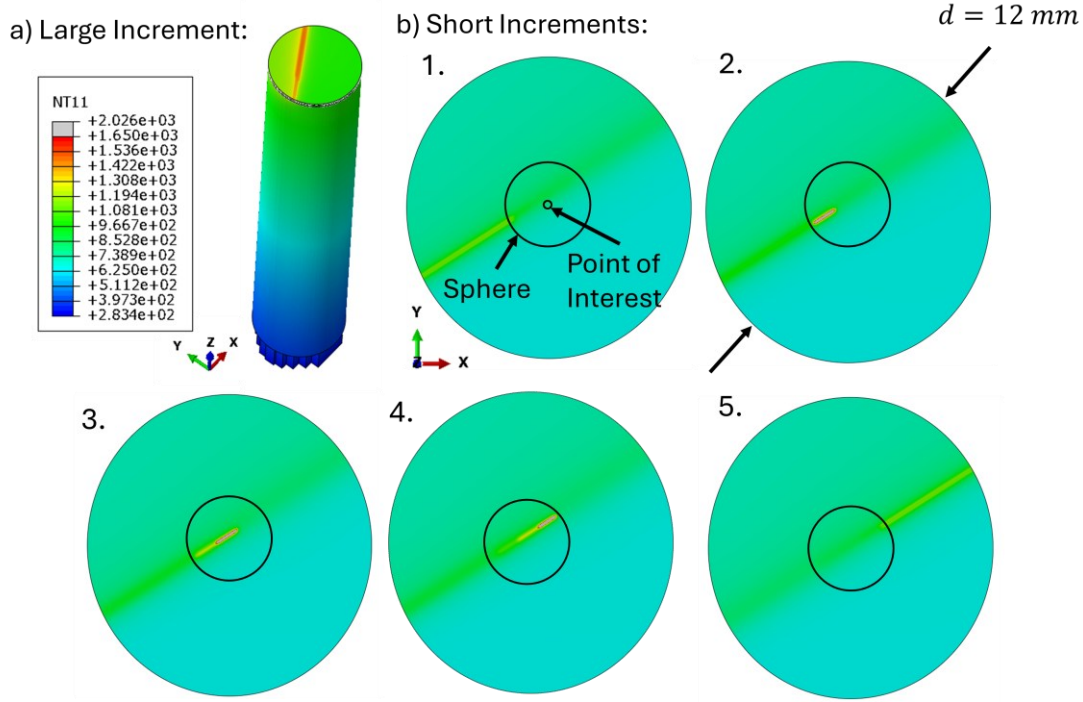


Figure 28. Visualisation of adaptive time increments used in the thermal FEA model, showing thermal contours in $^{\circ}\text{C}$ of a simulation printing a supported cylinder with 12 mm diameter and 100 mm height. **a)** Field output during a layer that did not interact with a sphere of interest, therefore having a large time increment. **b)** The top view of field outputs after different consecutive time increments in a layer which intersected a sphere of interest. The point of interest is located at the centre of the cylinder, which is shown in **1.**, together with an imaginary sphere surrounding it. **1.** shows the increment right before the laser enters the sphere of interest, **2.** **3.** and **4.** show progressive time increments when the laser is inside the sphere of interest (i.e., much shorter time increments to resolve the melt pool), and **5.** shows a larger time increment when the laser has exited the sphere of interest (i.e., about to re-enter again on return).

Therefore, the time stepping used during scanning uses 1ms increments inside of the spheres of interest, which have radii of 0.3 mm, and 60 ms increments outside. This is shown to be accurate through the experimental validation in the results of this chapter and the analysis in Appendix B.

Furthermore, time increments during cooling and recoating periods, when the laser is off, are increased to reduce computational time without a loss of accuracy. The time increments during recoating is set to 0.05s. During cooling time, the time increment is initially increased to 0.1s for 0.2s, and then further increased to 1s for the rest of the cooling period.

3.1.3 Thermal Properties

As explained in Section 2.3.1 - AM Process Thermal Models , thermal FEA simulations represent the powder, liquid, and solid phases as a single homogeneous solid. As a result, fluid dynamics, contact or convective interactions between phases are not explicitly modelled. To incorporate the thermal influence of each phase in the present work, phase-specific thermal material properties were used as suggested in ref. [81]. This was accomplished by adapting the specific heat capacity and thermal conductivity once the local temperature of the material reached the melting point, transitioning from the properties of the powder to those of fused Ti-6Al-4V. The transition of thermal properties at melting temperature is performed using the “Phase Transformations” utility in Abaqus. This utility tracks the temperature in all integration points with an internal subroutine and assigns a local field variable that simulates if the material is powder or fused. Then, material properties can be linked to this field variable to have dependence on the current phase of the material point. More information about the utility can be found in the Abaqus user manual.

The temperature-dependent heat capacity and thermal conductivity used for both the powder and fused Ti-6Al-4V are shown in Figure 29. These material properties were obtained from Simulia’s work in [81], which developed a similar FE simulation for LPBF of Ti-6Al-4V with experimental validation. The properties for the powder phase were taken to be a tenth of the fused material until it reaches melting temperature, when they are modified to converge towards the properties at the melting temperature of the fused alloy, which was set to $T_m = 1610^{\circ}\text{C}$.

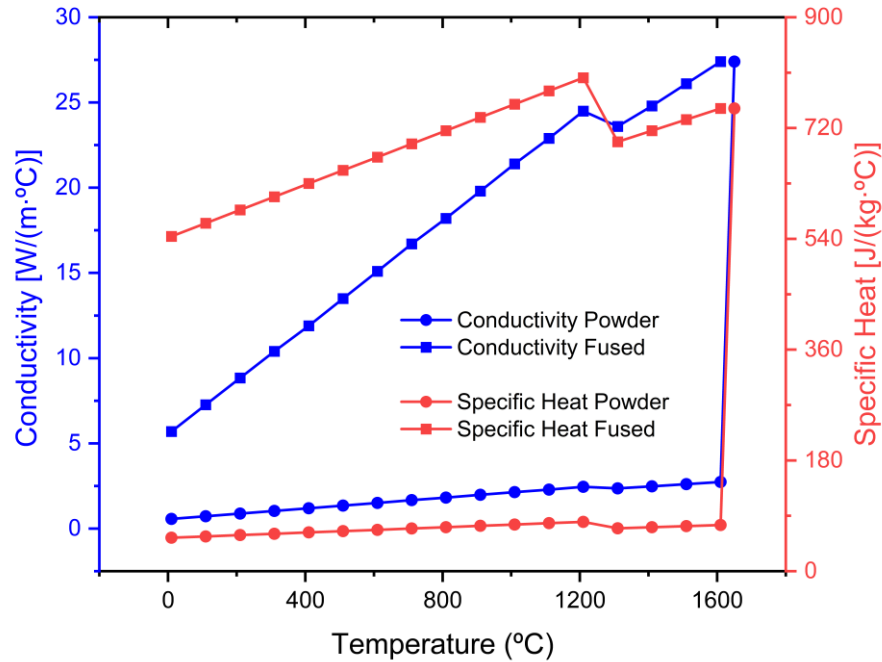


Figure 29. Temperature dependent thermal conductivity and specific heat capacity for both the powder and the fused Ti-6Al-4V material used in the thermal FE model. The properties considered for the powder were taken to be a tenth of the fused metal until it reaches the melting point, when it is modified to match those of the fused metal.

The effect of latent heats of fusion and evaporation have been neglected in this work. Although Abaqus offers models for their implementation, they introduce large non-linearities which lead to convergence problems without significantly affecting results at the temperature range of interest for metallurgical solid-state phase transformations.

Additional thermodynamic coefficients used for these simulations are provided in Table 1. An absorptivity value of $\alpha = 45\%$ was chosen for Ti-6Al-4V based on the measurements from ref. [115]. The density is assumed to be independent of temperature, as it changes moderately in contrast to k or c_p .

Table 1. Density and cooling properties used in the thermal AM model.

Density ρ	4430 kg/m^3
Emissivity ε	0.25
Convection Coefficient h	$18 \text{ W/(m}^2 \cdot \text{°C)}$
Absorptivity α	45 %

3.2 Experimental Validation Methods

The model has been validated using experimental temperature data, measured in-situ, from previous reports published in the literature. Two types of experiments were utilised. Firstly, data obtained by thermocouples embedded in the substrate plate, taken from Schnell et. al. in ref. [116], were compared to the simulation results. These experiments allow to ensure the model is correctly predicting the residual temperature that builds up and evolves during the entire process. Thereafter, to validate the temperature history around the melt pool, which drive phase transformations, the predicted temperatures were evaluated against data obtained via x-ray diffraction (XRD) indirectly (i.e., non-contact) by Chen et. al. in ref. [117]. These validation approaches allow to verify the results of predictive capabilities of the developed model both near the melt pool, and away from it for the entire AM process.

3.2.1 Validation by measurement with thermocouples embedded in substrate

Measuring temperature with thermocouples is a straightforward and common method to assess thermal phenomena (magnitude and distribution) during an AM process, and they are often used to validate FEA models. Ref. [116] studied heat buildup during LPBF using this technique. In their study, several geometries were printed while the temperature was measured in the substrate. A hole was drilled in the substrate plate to position the thermocouple 2 mm below the surface where the AM component was printed. The setup for these measurements is illustrated in Figure 30. Further information about the measurement procedure can be found in ref. [116].

To validate the thermal FEA model developed in this thesis, the AM process presented in ref. [116] was simulated taking into considerations all the relevant process parameters, and the temperature history was calculated at the nodes closest to the location of the thermocouple tip, see Figure 31. To simplify the FEA domain, the substrate was assumed as homogeneous, and the different holes and joints were not modelled, which is not expected to significantly affect the thermal history.

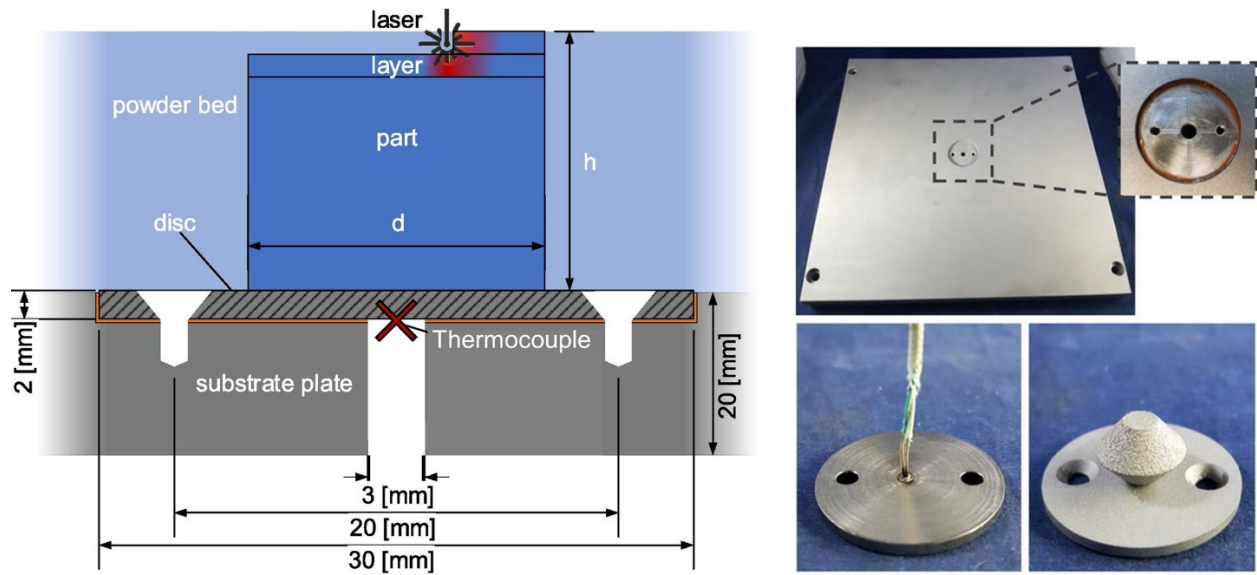


Figure 30. Illustration of the location of thermocouple installation from ref. [116] used to validate the thermal FEA model. The image in the left is a schematic of the process, showing the thermocouple located 2 mm below the centre of the printed part. The images in the right show photos of the setup. These images have been adapted from ref. [116].

The process parameters implemented in the simulation are provided in Table 2. The material used for printing in this experiment is EOSGP1 steel alloy, therefore the material properties were adapted. The thermal properties used were interpolated linearly with temperature; conductivity and specific heat values of $k = 13 - 46 \text{ W/m K}$ and $c_p = 0.44 - 0.83 \text{ J/g K}$ were used for the temperature range $T = 10 - 1610 \text{ }^\circ\text{C}$. These were obtained from ref. [116], which were calculated using the CALPHAD thermodynamic-based software. The absorptivity was set to $\alpha = 0.65$, which is a common value used for stainless steels [118].

Table 2. Process parameters used in the verification simulation with the experimental results obtained by thermocouple taken from ref. [116].

Process Parameters	
Scan Speed (v)	1150 mm/s
Laser Power (Q)	190 W
Laser Spot Radius (r)	50 μm
Layer thickness (t_{layer})	40 μm
Platform Temperature (T_{preheat})	Ambient – 26 $^\circ\text{C}$
Recoating time	9s
FOD	0 mm

The FEA model developed for one of the geometries tested can be seen in Figure 31. It shows the assembly and mesh used for one of the top layers. It also shows two field outputs with different views and the node where the temperature histories were extracted. The temperature histories were extracted at a node located in the same position as the thermocouple in the experiment, matching Figure 30. Since the thermal history was extracted from the substrate, i.e., away from the melt pool, a constant large time increment of 60 *ms* could be used while the laser was scanning, speeding up the simulation.

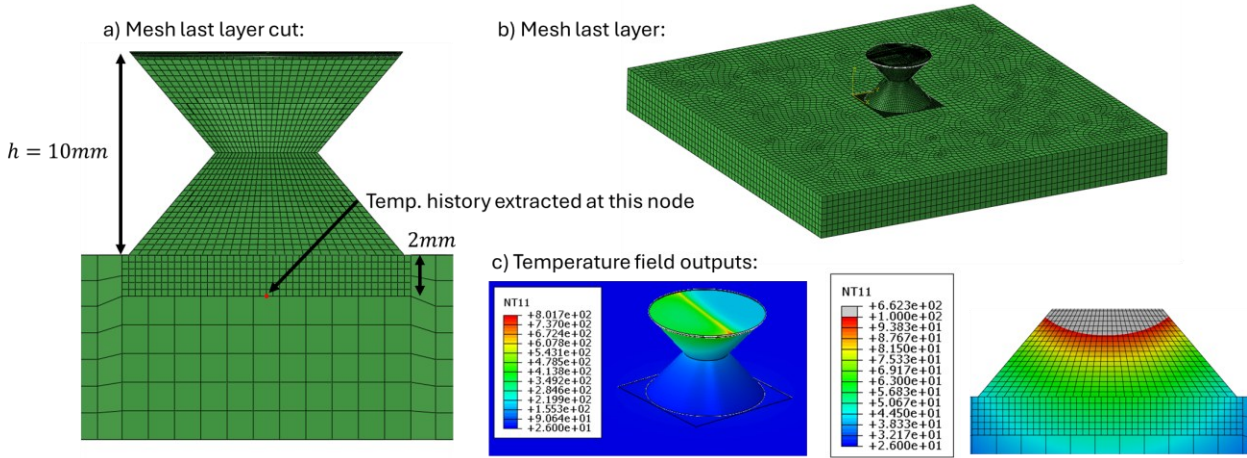


Figure 31. Mesh used and nodal temperature field outputs (in °C) of an FEA model for the experimental validation with thermocouples. **a)** Middle cut of the mesh around the printed geometry. It shows the node from where the temperature histories were extracted for validation, matching the position of the thermocouple experiment. **b)** Image of entire mesh. **c)** Temperature field outputs of the simulation at different stages and views. One of them is a view cut showing a smooth temperature transition at the substrate, demonstrating that the increased mesh size is appropriate there.

3.2.2 Verification by non-contact X-ray diffraction near the heat-source

Measuring thermal histories, in-situ, near the laser heated area, where phase transformation takes place during LPBF, is not a straightforward procedure. Thermocouples cannot be inserted close to the melt-pool due to high-temperature damage. Infrared imaging is useful to monitor the top layer and study the melt pool [119]; however, it does not provide information about temperatures in the layers below, where phase transformation occur. Recently, XRD has been proven to measure temperature, in-situ, in different layers at the proximity of the melt pool during LPBF of Ti-6Al-4V [117]. This method relates changes in the XRD profiles to the magnitude of temperature during the process.

The temperature measurements with XRD on LBPf of Ti-6Al-4V taken from Chen et. al. in ref. [117] have also been used to validate the result of the thermal model developed in this thesis. Using the non-contact XRD measurement method, the authors reported the temperature at several layers below the surface while the top layer was being scanned. They used high-speed XRD, in-situ, in transmission mode and probed different layers during the printing of a thin wall. By measuring the peak shifts in the diffraction patterns caused by isotropic thermal expansion, the magnitude of the temperature could be evaluated. Further information about the measurement procedure can be found in ref. [117]. A schematic of the measurement and the results are shown in Figure 32.

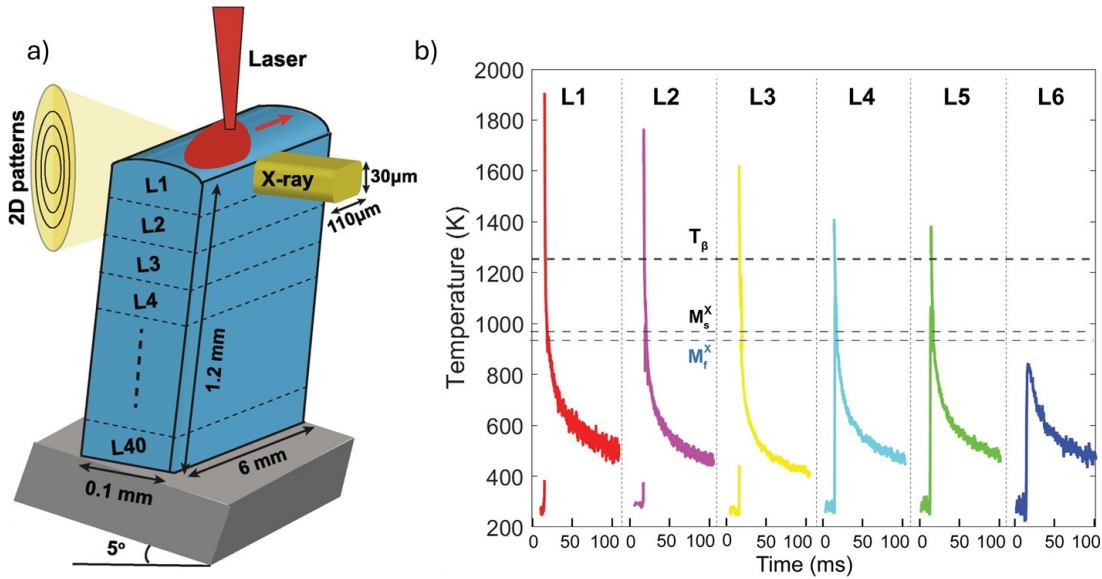


Figure 32. **a)** Schematic of the XRD method for the measurement of temperature, in-situ, during LPBF. It shows a thin wall being probed with an X-ray beam as the top layer is being scanned. **b)** The temperature profiles measured for each layer by XRD at the top 6 layers while the top layer is being scanned. Figure adapted from ref. [117].

The process parameters used in the measurement trials are provided in Table 3. A thin wall was manufactured containing a single laser track per layer, represented in Figure 32.a). The dimensions of the printed wall were $6 \times 1.2 \times 0.1 \text{ mm}^3$. The thin wall consisted of 40 layers and the XRD measurements were performed at the top 6 layers. The measurements for each layer were performed one at a time while the top layer was rescanned.

Table 3. LPBF process parameters used during the in-situ XRD temperature measurements in ref. [117], which has been used to validate the thermal FE model developed in this work.

Process Parameters	
Scan Speed (v)	600 mm/s
Laser Power (Q)	100 W
Laser Spot Radius (r)	23.5 μm
Layer thickness (t_{layer})	30 μm
Platform Temperature (T_{preheat})	Ambient – 26 $^{\circ}\text{C}$
FOD	0 mm

To validate the thermal FE model developed in this work, an identical simulation of the LPBF process carried out during these measurements was created, as shown in Figure 30.a). Thereafter, the temperature histories were extracted at the same positions which were probed by the XRD beam, as shown in Figure 30.b). The temperatures at 4 different elements in the same layer were averaged for the thermal results of each layer, which approximates the area of probing of the X-ray beam seen in Figure 29. As opposed to the validation with the results of thermocouple measurements of the previous section, in this simulation the thermal histories were extracted adjacent to the heat source. This required a high-resolution time discretisation, therefore a short time step of 1 ms was used for this simulation.

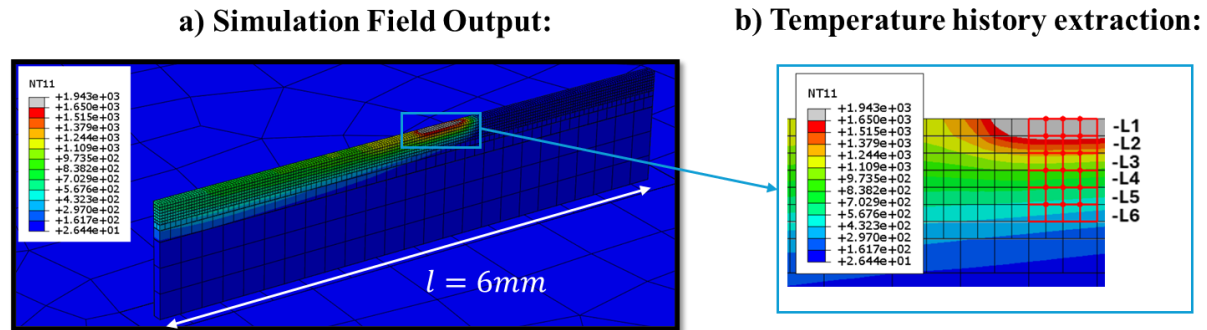


Figure 33. **a)** Field output of thermal FEA simulation showing the thin wall on top of the substrate while the laser is scanning the top layer. The melt is coloured in grey. **b)** Zoomed-in side view of the melt pool; the elements marked with the red grid are those from which the temperatures were extracted and averaged for every layer. Each analysed layer contains one element through its height. Additional geometrical information given in Figure 32.a).

3.3 Results

3.3.1 Validation of the thermal FEA model with thermocouple measurements

The results of the FE simulation were compared with the experimental data from the thermocouple measurements (i.e., reported in ref. [116]) and the outcome is illustrated in Figure 34. The plotted value θ corresponds to the temperature difference between the measured temperature and the ambient temperature ($\theta = T - T_{amb}$), with the ambient temperature being $T_{amb} = 26^\circ\text{C}$ as explained in the methodology. The plots, as expected, show many peaks, which correspond the heatwaves generated by printing each layer. This is because the thermal history for the entire process is being reported, which consists of many layers. The simulated thermal histories show good agreement with the experiments both in terms of the temperature peaks and the residual heating along the whole process for the different geometries. This proves that the thermal FEA model is accurate in capturing the geometrical effects on temperature for different parts. Since large time increments were used for these simulations, it also shows that large time discretisation and mesh refinement can be used to accurately capture thermal histories away from the heat source.

Nonetheless, some deviations in the results can be appreciated which have been attributed to uncertainties in both the experimental procedure and the FEA model. The modelling uncertainties arise from the different assumptions taken regarding the thermal material properties, heat source and cooling parameters. The thermal properties of the material were linearly interpolated with temperature based on CALPHAD simulation results; more accurate thermal properties from experimental measurements could improve accuracy. The heat source parameters used in the Goldak model were approximated based on the laser process parameters. It would be more precise to calibrate them based on experimental measurements of single bead experiments [120] or CFD simulations [51]. This also affects the cooling parameters like the convection coefficient or the boundary conditions, which depend on airflow and change depending on a specific AM machine and should theoretically be calibrated. Nonetheless, with more appropriate calibration, it is shown here that this model has the potential to compute heat build-up with high precision, which is a critical physical phenomenon with high impact on the final material (residual stress, melt-pool stability, microstructure, etc).

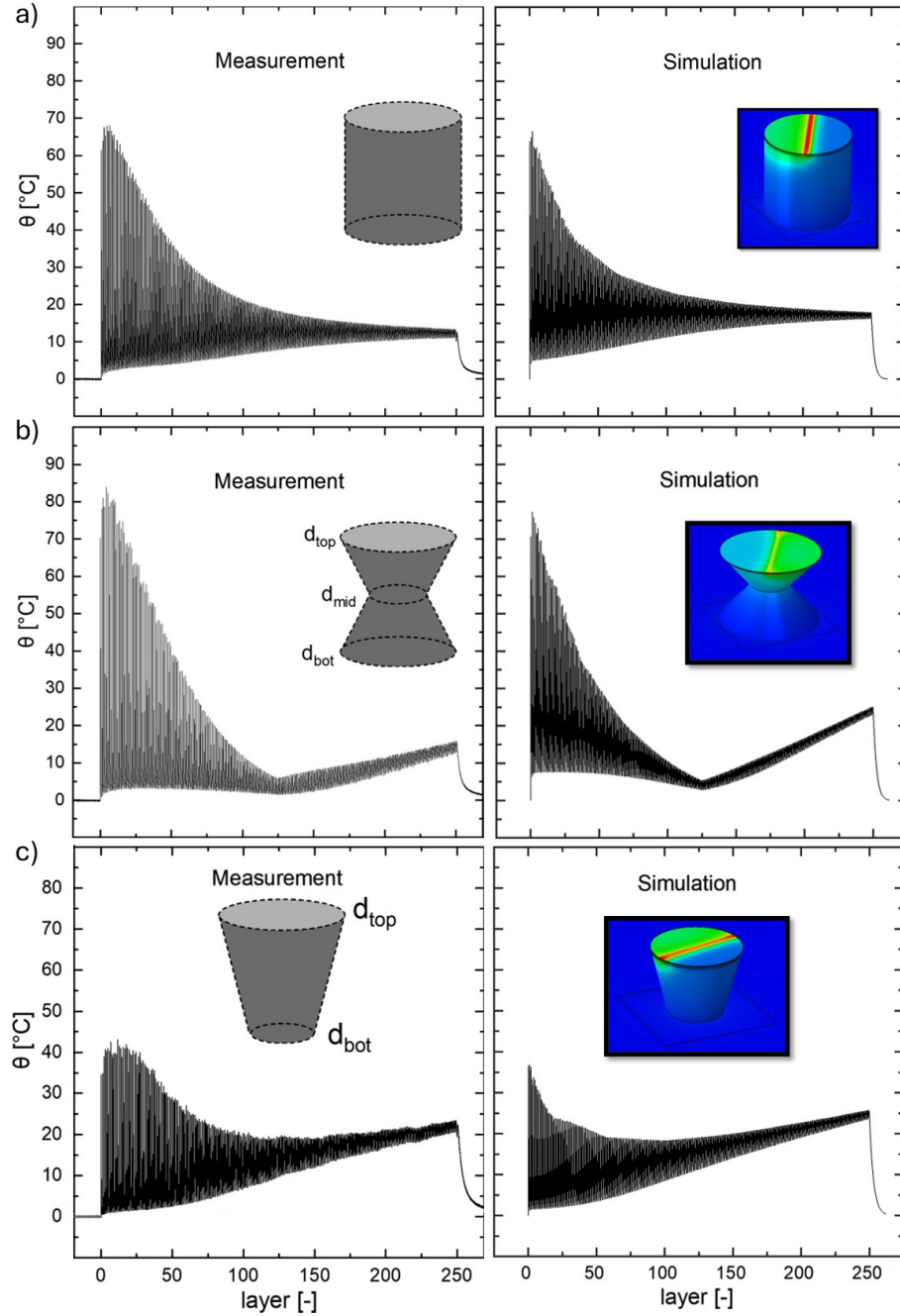


Figure 34. Comparison between thermal histories measured by thermocouples and those predicted by the developed thermal FEA model for different geometries, all with a height of $h = 10 \text{ mm}$. The plotted value θ refers to the temperature difference with the ambient temperature ($\theta = T - T_{amb}$). **a)** A cylinder with a diameter of $d = 10 \text{ mm}$, **b)** an hourglass shape with $d_{top/bot} = 13.5 \text{ mm}$ and $d_{mid} = 5 \text{ mm}$, and **c)** a cone with $d_{bot} = 5 \text{ mm}$ and $d_{top} = 10 \text{ mm}$. The simulation graphs include a field output of the model while the last layer is being scanned. The thermocouple measurement graphs have been adapted from ref. [116].

3.3.2 Validation of the thermal FEA model with XRD temperature measurements

Figure 35 shows the comparison of the thermal FEA model predictions and the XRD temperature measurements (i.e., non-contact) from ref. [117]. The comparison between the temperature values of the experiment and the simulation can be seen in Figure 35.c). These show the different heat waves experienced at each of the top six layers while the top layer is being printed. There exists some deviation in the peak temperatures, which can be attributed to uncertainties in both the experimental method and modelling parameters, and are discussed in more detail in the discussion section (Section 3.3.3). However, peak temperatures will have a low effect on predicting phase fractions since the time at these high temperatures is very short. On the other hand, the predicted cooling rates seem to agree well with the experimental results, which are more influential in determining the solid-state phase transformations that happen during AM of Ti-6Al-4V [26].

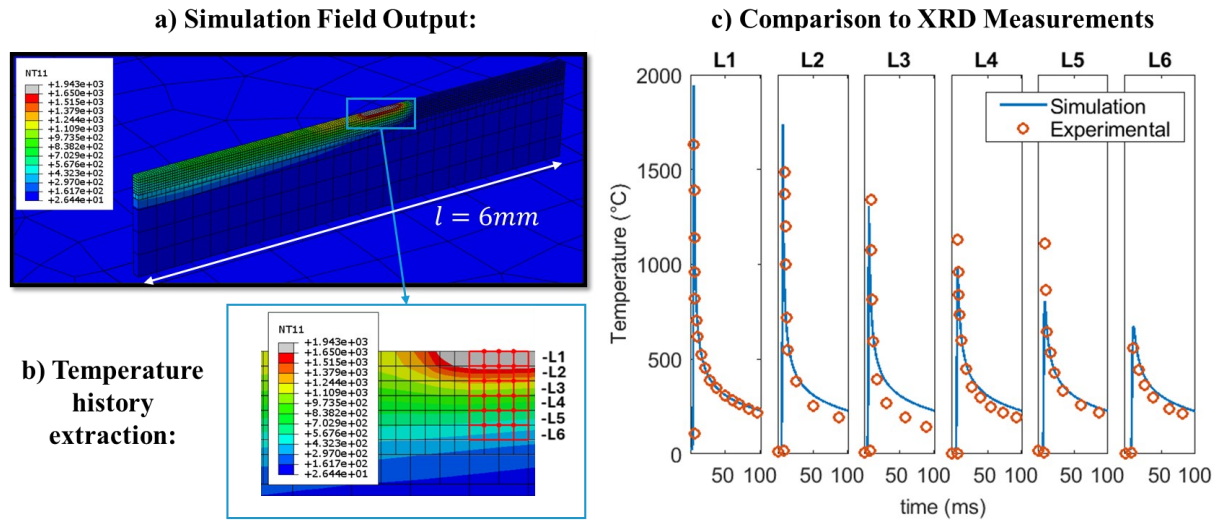


Figure 35. **a)** Field output of thermal FEA simulation showing the thin wall on top of the substrate while the laser is scanning the top layer. **b)** Zoomed-in side view of the melt pool; the elements marked with the red grid are those from which the temperatures were extracted and averaged for every layer. Each layer contains one element through its thickness. **c)** Comparison between the temperature histories measured by XRD and those predicted by the thermal FEA model. Additional geometrical information given in Figure 32.a).

3.3.3 Discussion and Conclusions

The developed thermal FEA model has proven successful in calculating thermal histories both near and far from the heat source while capturing the effect of different geometries, materials, and process parameters. As opposed to lumped sum approaches that are currently used for residual stress measurements, the proposed modelling approach yields high-resolution thermal histories throughout the whole process, which is needed to predict microstructural phase transformations.

This is made possible by the adaptive spatial and time discretisation proposed in this work, which allow to model each geometry of Figure 34 in approximately 2 hours using 8 Intel Xeon Gold 6138 CPUs, as opposed to weeks if static meshing and constant time increments were used. It must be noted that the achieved computational speed is a step in the right direction and allows to use this model for design validations; however, this approach is not fast enough for it to be used in optimisation algorithms for topology or process parameter optimisations. Some possible approaches to achieve this speed could be analytical models [56], better adaptive discretisation approaches using open-source FEA libraries [112] or acceleration with machine learning surrogates [121]. Analytical models can yield much faster solutions but need to make certain assumptions that can decrease their accuracy. Open-source FEA libraries, such as deal.II [113], allow to freely perform adaptive mesh refinement in a much more optimized manner than what is achievable currently with commercial FEA software, but development time can be much higher. Finally, machine learning surrogates are gaining a lot of attention by accelerating simulations using data-driven models trained on the results of the simulations themselves. However, it is also a complex process that requires significant resources, development time and benchmarking. A combination of these approaches is likely to enable the iterative use of thermal models within optimisation routines, thereby allowing automatic optimisation of process parameters or geometry. Overall, the authors expect that the results presented in this thesis demonstrate that thermal FEA models of AM hold significant potential for such applications and incentivize further research in accelerating them.

On another note, the author acknowledges that deviations exist between the computed temperature histories and the experimental measurements. Although part of these deviations could be attributed to imprecisions during the experimental methods, important modelling assumptions have been made to carry out the comparisons with the literature presented here. Most uncertainties in the model could be mitigated by calibrating the model to a specific machine and material.

Goldak parameters could be better calibrated by matching the melt pools during single scan experiments [122]. The thermal properties used for EOSGP1 could be measured with higher fidelity. Cooling parameters like convection coefficients can be machine and material dependent and could be calibrated to better match experimental thermal measurements like in ref. [123]. Additionally, absorptivity coefficients can be measured for specific laser configurations and materials instead of being assumed constant, as done in ref. [120]. For industrial application of this model, it is likely that the model parameters need to be fine-tuned for different machines and materials. However, it may be possible to automate these calibrations, which could perhaps be offered by the AM machine vendor.

Despite the assumptions adopted, overall, the developed model provides sufficiently accurate predictions of cooling rates and residual heating to assess metallurgical evolution in relation to geometry and process parameters, which was the main aim for the thermal model in this thesis. The following chapters analyse how the temperature histories from this thermal model can be used as input to a microstructure evolution model to predict the resulting microstructure and properties of Ti-6Al-4V.

4. MICROSTRUCTURE EVOLUTION MODEL OF TI-6AL-4V DURING POWDER-BED ADDITIVE MANUFACTURING

Since a process model capable of yielding accurate temperature histories has been developed in **Chapter 3**, the next step in the PSPP chain is to calculate microstructure evolution for a given temperature history during the AM process. There are several techniques being used to model the chemical and morphological evolution of metallic polycrystals during manufacturing processes [65, 66]. Some common approaches to simulate the microstructure evolution include Front-Tracking [71], Phase-Fields [124-128], Cellular Automaton [76, 77], Level-Set [129, 130] and Kinetic Monte Carlo [72, 73] simulations. These full-field approaches represent the microstructural dynamics of solidification and phase transformation spatially using physically based numerical methods. However, these methods are computationally expensive, and many different simulations would be required for the PSPP modelling in AM of Ti-6Al-4V. For this reason, a model to predict all the phase transformations during AM of Ti-6Al-4V has not yet been reported in the literature using full-field methods.

Instead, analytical mean-field models develop estimates of microstructural transformations using only scalar temperature history. Although limited in physical fidelity with regards to the previously explained methods, they can be easily integrated into thermal FEA codes to calculate microstructural features at each integration point while the FEA simulation runs. This allows to couple the FEA simulation with the microstructural information calculated to account for additional physical effects on thermal and structural behaviour [77, 128, 131-136]. This chapter summarises the development of a mean-field model to track phase transformation in Ti-6Al-4V during powder-bed AM process, and validates its prediction capability experimentally.

4.1 Modelling Methodology

The developed model reads a temperature history in the form of tabular data and uses a combination of analytical equations in incremental form to calculate the most influential phase fractions and grain morphologies on the strength of the final Ti-6Al-4V product. It has been developed as a Python library that can read temperature histories from a CSV file and calculates microstructure evolution for the entire time history provided, yielding the outputs as graphs and

CSV files. A link to a repository with the code can be found in Appendix A.2. The main objective is to use this model with the temperature histories provided by the thermal FEA model of **Chapter 3**, but the model would also work with temperature histories obtained with other methods, like thermal measurements with thermocouples.

4.1.1 Volumetric Phase fractions Calculation

Following the work presented in [81], the developed framework defines phase transformation in a given material based on parent-children relationships, where p denotes the parent phases and c_i denotes the child phases:

$$p \rightarrow c_1 + c_2 + \dots + c_n \equiv p \rightarrow c \quad \text{Equation 5}$$

For every time increment of the input thermal history, if the conditions for a given transformation are met in terms of temperature (T), heating/cooling rate (dT/dt) and current phase fractions (f_n), a transformation in this time increment is calculated that changes the values of the current phase fractions. The different possible transformations are modelled either as diffusional transformation based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model [137] or as displacive based martensitic based on the Koistinen-Marburger (KM) model [138], with the corresponding coefficients varying depending on the specific transformation. These coefficients can be calculated from isothermal time-temperature-transformation (TTT) diagrams. TTT diagrams can be measured experimentally or calculated using programs like Thermo-Calc or JMatPro.

For diffusional transformations, since additive manufacturing involves non-isothermal heating and cooling, the classic JMAK equation has been extended as in ref. [139] to consider continuous temperature variation as a series of small consecutive isothermal steps. The equation used is displayed in Equation 6, where $f_p(T + \Delta T)$ is the parent phase fraction at the end of the current temperature change; and k and n are the JMAK coefficients, which can be calculated from TTT diagrams. For the diffusional transformations to occur, the volume fraction of the parent phase must follow $f_p > f_{tot} f_{p,0}^{eq}$, as the phases are transforming to reach the equilibrium phase fractions following to the phase diagram. In this inequality, $f_{p,0}^{eq}$ is the equilibrium phase fraction

of the parent phase in the mixture that only contains parent and child phases of the given transformation; and f_{tot} is the sum of the phase fractions accounted in the current transformation ($f_{tot} = f_p + f_c$). The multiplication $f_{tot}f_{p,0}^{eq}$ allows this equation to work in the case of the material containing more phases than the ones participating in the current diffusional transformation. It basically normalizes the ideal binary equilibrium fraction $f_{p,0}^{eq}$ against the total volume of the active phases f_{tot} , which calculates the absolute thermodynamic target for the parent phase across the heterogeneous alloy.

$$f_p(T + \Delta T) = f_{tot} \left(1 - (1 - \exp[-k(\xi + \Delta t)^n])(1 - f_{p,0}^{eq}) \right), \text{ if } f_p > f_{tot}f_{p,0}^{eq} \quad \text{Equation 6 a}$$

$$\xi = \left[-\frac{1}{k} \ln \left(\frac{f_p(T) - f_{tot}f_{p,0}^{eq}}{f_{tot}(1 - f_{p,0}^{eq})} \right) \right]^{1/n} \quad \text{Equation 6 b}$$

If a diffusional transformation is reversible, the reverse transformation is calculated as:

$$f_p(T + \Delta T) = f_{tot}(1 - \exp[-k(\xi + \Delta t)^n])f_{p,0}^{eq}, \quad \text{if } f_p < f_{tot}f_{p,0}^{eq} \quad \text{Equation 7}$$

In the case of a diffusional transformation having several child phases, their phase fractions are calculated referring to their equilibrium phase fractions using Equation 8:

$$f_{c_i}(T + \Delta T) = f_{c_i} + (f_p - f_p(T + \Delta T)) * f_{c_i,eq} \quad \text{Equation 8}$$

For displacive or martensitic transformations where no diffusion is expected to take place, they are modelled to solely depend on temperature according to the KM equation [139], as they are shown as straight lines in TTT diagrams:

$$f_c(T) = f_c(T_0) + (f_p(T_0) - f_{pr})(1 - \exp[-\gamma(M_s - T)]) \quad \text{Equation 9}$$

Due to the arbitrary thermal histories in AM, a backward Euler integration in differential form of the original KM model developed in ref. [135] is used, displayed in Equation 10. Furthermore, martensitic transformations are set to occur only if the volume fraction at the start of cooling $f_p(T_0)$ is higher than the retainable amount of parent phases f_{pr} . This is to model the effect of different chemical composition at different phase fractions, which affects phase transformations. For example, in the transformation of $\beta \rightarrow \alpha'$ in Ti-6Al-4V, β contains higher Vanadium at lower phase fractions, which limits the transformation of β to α' if f_β is low enough [140], retaining some β after the transformation.

$$f_c(T + \Delta T) = \frac{f_c(T) - \gamma \Delta T (f_p(T_0) - f_{pr} + f_c(T_0))}{1 - \gamma \Delta T}, \quad \text{if } f_p(T_0) > f_{pr} \quad \text{Equation 10}$$

For this work, several different transformations have been defined for Ti-6Al-4V in powder-bed fusion processes using the previously explained equations. All the transformations modelled are displayed in Table 4 and explained in the following paragraphs.

Table 4. Transformations included in the microstructure evolution model for Ti-6Al-4V during additive manufacturing. The table states the type of mathematical model used for each transformation and the necessary conditions for it to happen.

Transformation		Type	Occurring Conditions	
1	$\beta \rightarrow \alpha'$	Martensitic (KM)	Fast cooling ($\dot{T} < -20^\circ\text{C/s}$) and $T \leq T_{Ms} = 851^\circ\text{C}$	$f_\beta > f_{\beta_r}$
2	$\alpha' \rightarrow \alpha + \beta$	Diffusional (JMAK)	Heating ($\dot{T} \geq 0^\circ\text{C/s}$) and $T > T_{diss} = 400^\circ\text{C}$	$f_{\alpha'} > f_{\alpha',0}^{eq}$
3	$\beta \rightarrow \alpha$		Slow cooling ($0 > \dot{T} > -20^\circ\text{C/s}$)	$f_\beta > f_{\beta,0}^{eq} * (f_\alpha + f_\beta)$
3R	$\alpha \rightarrow \beta$	Diffusional (Parabolic)	Heating ($\dot{T} \geq 0^\circ\text{C/s}$)	$f_\beta < f_{\beta,0}^{eq} * (f_\alpha + f_\beta)$

Upon solidification, when the material cools below melting temperature ($T_{melt} = 1610^\circ\text{C}$), it consists fully of BCC β phase, therefore the volumetric phase fraction of β is set to $f_\beta = 1$. Depending on the cooling rate, β can then transform into the acicular needle-like metastable HCP martensitic phase (α') for fast cooling rates through a martensitic transformation ($\beta \rightarrow \alpha'$) or into lamellae of the HCP α -phase (α) through a diffusional transformation ($\beta \rightarrow \alpha$).

Therefore, the former is modelled with the KM equations and the latter with the JMAK formulation.

Furthermore, the heat induced by the laser passing through nearby regions can induce two further diffusional transformations. These are the decomposition of α' into a mixture of $\alpha + \beta$ ($\alpha' \rightarrow \alpha + \beta$) if temperature is higher than the martensite dissolution temperature ($T_{diss} = 400^\circ\text{C}$); as well as the dissolution of α into β ($\alpha \rightarrow \beta$). The $\alpha' \rightarrow \alpha + \beta$ transformation is modelled using the JMAK equations. However, for the $\alpha \rightarrow \beta$ transformation, a parabolic growth model has been used. Although this transformation could theoretically be modelled using a reverse transformation of $\beta \rightarrow \alpha$ with the JMAK model, the parabolic grain growth model displayed in

Equation 11, where T is in Kelvin, has been shown to better represent the kinetics in this transformation [81, 82, 141]. This is because the $\alpha \rightarrow \beta$ transformation is a dissolution process, while JMAK is fundamentally designed for nucleation and growth processes. The phase transformations modelled were explained in more detail in the literature review (**Chapter 2.2.2**).

$$f_\alpha(T + \Delta T) = \begin{cases} 1 - f_\beta^{eq}(T + \Delta T)f_{diss}(T)\sqrt{\Delta t + t^*} & \text{if } 0 < \Delta t + t^* < t_{crit} \\ 1 - f_\beta^{eq}(t + \Delta t) & \text{if } \Delta t + t^* \geq t_{crit} \end{cases} \quad \text{Equation 11 a}$$

$$t^* = \left(\frac{f_\beta(T)}{f_\beta^{eq}(T + \Delta T)f_{diss}(T)} \right)^2 \quad \text{Equation 11 b}$$

$$t_{crit} = f_{diss}(T)^{-2}, \quad f_{diss}(T) = 2.2 * 10^{-31} * T^{9.89} \quad \text{Equation 11 c}$$

As explained, besides the cooling rate and temperature requirements, a given transformation only occurs if certain values of current parent phase fractions are present in the material. For Martensitic transformations, the fraction of the parent phase (f_p) must be larger than the fraction of its retainable phase fraction (f_{p_r}), which for β it is assumed to follow the relationship expressed in Equation 12 [135].

$$f_{\beta_r} = \begin{cases} f_\beta(T_0), & f_\beta(T_0) < 0.25 \\ 0.25(1 - f_\beta(T_0)), & f_\beta(T_0) \geq 0.25 \end{cases} \quad \text{Equation 12}$$

For diffusional transformations to occur, the parent phase must be higher than its equilibrium fraction in the mixture of phases that are considered in the transformation ($f_p > f_{tot} f_{p,0}^{eq}$). The temperature dependent values of $f_{\alpha',0}^{eq}$ and $f_{\beta,0}^{eq}$ are displayed in Figure 36.a), obtained from [81]; $f_{\alpha,0}^{eq}$ is calculated as $f_{\alpha,0}^{eq} = 1 - f_{\beta,0}^{eq}$. For the martensitic transformation, the transformation start temperature and transformation coefficient are needed, which are set to $M_s = 851$ °C and $\gamma = 0.015$ °C⁻¹, respectively, obtained from [142]. Finally, the JMAK coefficients for the diffusional transformations are required, all which are displayed in Figure 36. The JMAK coefficients for $\beta \rightarrow \alpha$ were obtained from ref. [143], while the coefficients for $\alpha' \rightarrow \alpha + \beta$ were obtained from ref. [82]. Unfortunately, the source data lacks error bars; an analysis on the variability of these inputs and a formal uncertainty quantification of the simulation outputs in the future would be beneficial to improve the robustness of the model.

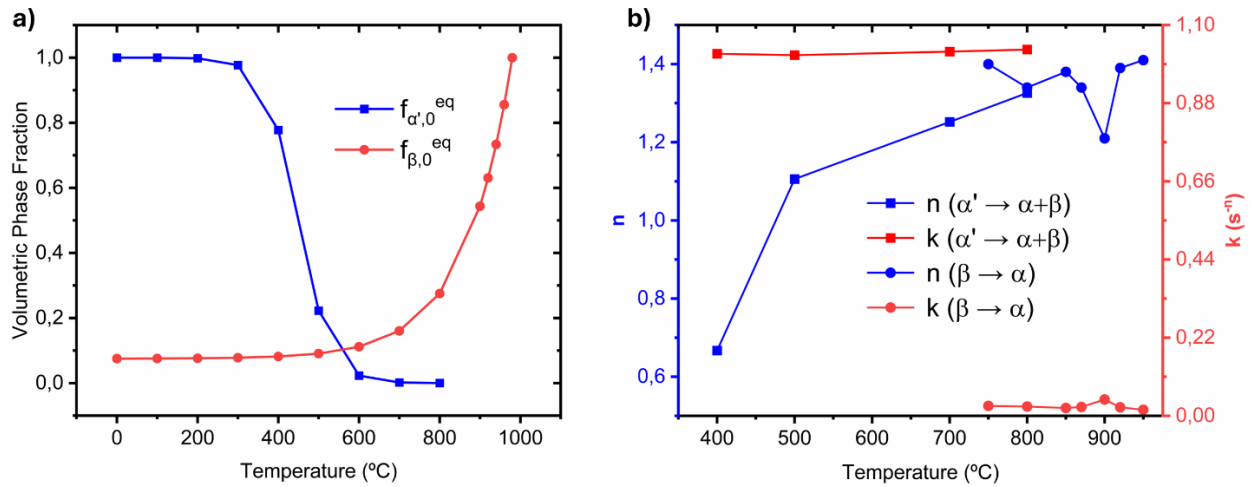


Figure 36. Material properties used in the diffusional phase transformations $\beta \rightarrow \alpha$ and $\alpha' \rightarrow \alpha + \beta$. **a)** Equilibrium volume fractions of the parent phases in the mixture that only contain the parent and children phases involved in a given transformation. **b)** JMAK coefficients for the diffusional transformations used in the MEM.

A flow-chart of the algorithm developed is displayed in Figure 37. The flowchart shows the process to calculate the changes in phase fractions for each time increment of the given thermal history.

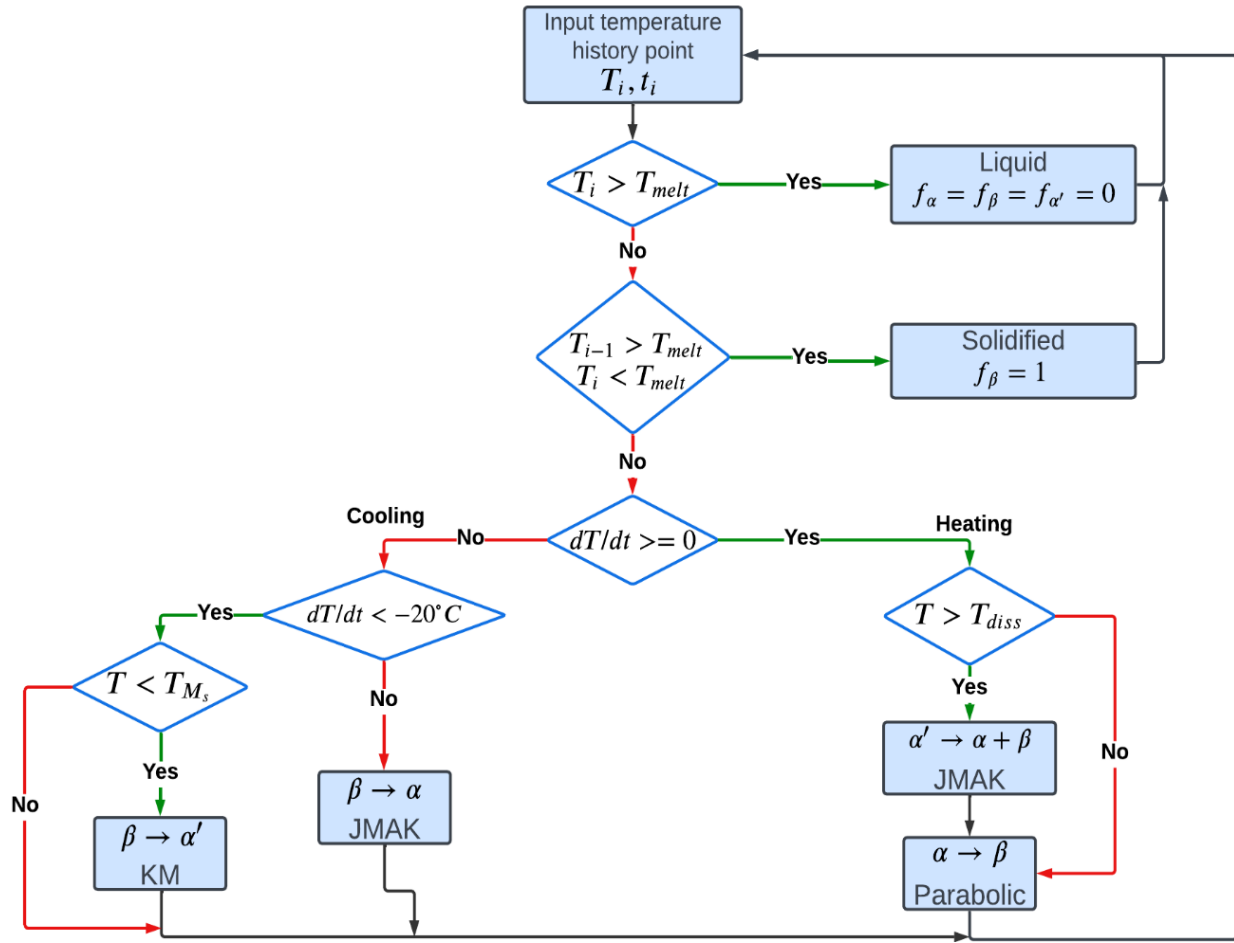


Figure 37. Flowchart of the algorithms used to calculate changes in phase fractions for each time increment of the microstructure evolution model.

4.1.2 Grain Morphology Calculation

Furthermore, besides phase fractions, further analytical equations based on temperature have been proven to yield reliable estimates of the morphological features that mainly influence mechanical properties [81]. These grain morphology calculations have been added to the mean-field model and are carried out in each time increment after calculating the phase fractions.

For the case of Ti-6Al-4V, the diameter of the parent β grains can be calculated using the parabolic grain growth law shown in Equation 13 when the temperature is between β -transus and the solidus temperature [144]. This equation models the grain growth of β by reduction of grain boundary energy. Values of $n = 2$ and $k = 2.2\text{m}^2/\text{s}$ were used for the coefficients, and $Q = 251\text{kJ/mol}$ was set for the activation energy of the β phase. $R = 8.314\text{J}/(\text{mol} \cdot ^\circ\text{C})$ is the

universal gas constant. The initial β grain size is assumed to be equal to the hatch spacing, which is an estimate of the width of the melt pool.

$$d_{t+\Delta t}^n = d_t^n + \Delta t k \exp\left(-\frac{Q}{R(T - T_x)}\right) \quad \text{Equation 13}$$

The elongation of the β grains can be predicted from experimentally measured solidification maps, as shown in Figure 38 [144], which uses the thermal gradient G and solidification rate $R = \left|\frac{\dot{T}}{G}\right|$ to determine if the β grains will be columnar, equiaxed or mixed.

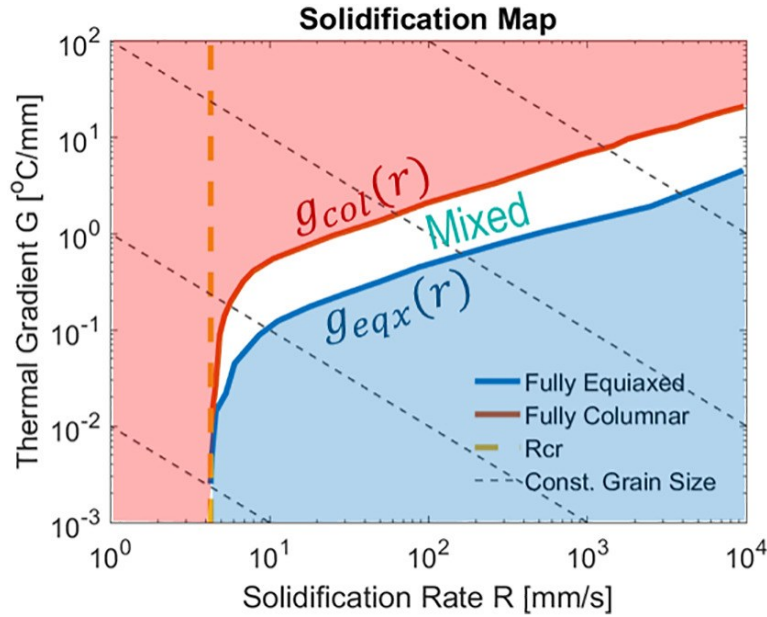


Figure 38. Experimental solidification map for β grain morphology prediction, relating its dependence on thermal gradient G and solidification rate $R = \left|\frac{\dot{T}}{G}\right|$. Each line separates regions in the map where different β grain morphologies are expected. The red region above and left of the g_{col} curve corresponds to solidification conditions that will yield a columnar microstructure. The blue region below g_{eqx} will produce equiaxed maps, and the mixed region will yield a mix of the two morphologies. Figure reproduced from ref. [144].

Finally, the average thickness of α laths has also been shown to be predicted by temperature according to an empirical Arrhenius equation in the incremental form [145], which is shown in Equation 14. The initial t_{lath} has been set to $0.25 \mu m$, the Arrhenius prefactor to $k_{lath} = 0.45 \mu m$ and the activation temperature $R_{lath} = 294 K$.

$$t_{\alpha}^{eq} = k_{lath} * e^{\frac{-R_{lath}}{T}} \quad \text{Equation 14 a}$$

$$t_{\alpha}(t + \Delta t) = t_{\alpha}(t) * \frac{f_{\alpha}(t)}{f_{\alpha}(t+\Delta t)} + t_{\alpha}^{eq} * \left(1 - \frac{f_{\alpha}(t)}{f_{\alpha}(t+\Delta t)}\right) \quad \text{Equation 14 b}$$

This equation models the kinetics of α growth against a change in β at different temperatures using the phase fractions predicted by the JMAK model through a weighted average approach. Therefore, it also accounts for the effect of cooling rate. However, to also consider the α grain growth by reduction of interfacial energy (classic grain coarsening kinetics [146]), which can be significant in long AM processes for large components or heat treatments, a parabolic grain growth term has been added in this work. Values of $k_{GB} = 19 \text{ m}^2/\text{s}$, $Q = 97 \text{ kJ/mol}$ and $c = 3$ were obtained initially from ref. [147] and then fitted to match the experimental results. The final equation for α lath thickness prediction is displayed in Equation 15, where the parabolic grain growth is applied to an intermediate value ($t_{\alpha_{int}}$) calculated using Equation 14.

$$t_{\alpha}^{eq} = k_{\alpha} * e^{\frac{-R_{lath}}{T}} \quad \text{Equation 15 a}$$

$$t_{\alpha_{int}} = t_{\alpha}(t) * \frac{f_{\alpha}(t)}{f_{\alpha}(t+\Delta t)} + t_{\alpha}^{eq} * \left(1 - \frac{f_{\alpha}(t)}{f_{\alpha}(t+\Delta t)}\right) \quad \text{Equation 15 b}$$

$$t_{\alpha}(t + \Delta t) = \sqrt[c]{t_{\alpha_{int}}^c + k_{GB} * e^{\left(-\frac{Q}{RT}\right)t}} \quad \text{Equation 15 c}$$

Once t_{α} is known, assuming a repeating lamellar unit cell structure, the lath thickness of β (t_{β}) has been calculated in this work through Equation 16. Regarding martensitic α' , $t_{\alpha'}$ is not calculated in this work, since its morphology after formation is hard to predict and not affected by the subsequent thermal history. This is because it decomposes into α and β before any coarsening occurs [148].

$$t_{\beta} = t_{\alpha} * \frac{f_{\beta}}{f_{\alpha}} \quad \text{Equation 16}$$

Since this thesis focuses on a PSPP model for yield strength, with regards to morphology, only the lath thicknesses will be analysed in this work, as the size and shape of the parent β grains (PBGs) have been shown not to have a significant effect on strength of Ti-6Al-4V, i.e., affecting mostly ductility and fatigue [12]. By calculating the phase fractions and the lath thickness, the developed analytical model for microstructural evolution can yield a quantitative estimate of the average microstructural values that have the most influence on the strength of AM built Ti-6Al-4V.

4.2 Experimental Validation

Firstly, the developed microstructure evolution model has been validated using in-situ phase fraction measurements from Babu et. al. [149] obtained using high-speed XRD measurements during a power based laser Directed Energy Deposition (DED) process. Ideally, a LPBF process would be used for the validation as they tend to produce different heating and cooling rates, but none have been reported so far to the knowledge of the author. The authors reported the temperature history and α and β phase fractions during several layers. The experimental thermal history reported was used as input for the model and the phase fraction calculated was contrasted with the measured values. However, the XRD measurements did not allow to distinguish between α' and α and only studied a small period of the time history during the process.

Alternatively, the model has also been validated by comparing its microstructural predictions with measurements from Scanning Electron Microscopy (SEM) micrographs. This was performed for the samples built via LPBF under different process parameters at several positions along the printed components. Experimental micrographs from both in-house experiments and the literature have been used. To obtain the entire thermal histories of the process at the different analysed positions, the AM process for each build was simulated using the thermal model from **Chapter 3**. Then, the thermal histories calculated were input into the MEM to obtain the phase fractions and lath thicknesses at these positions. The predicted values are contrasted with experiments by quantitative image analysis of Backscatter Electron (BSE) images that quantified the microstructures in the experimental samples.

4.2.1 In-House Powder-bed AM and Material Characterisation

Small cuboids of Ti-6Al-4V were printed using a RenAM 500S machine using the Reduced Build Volume (RBV) configuration. The RBV configuration allows to manufacture small builds with a much lower amount of powder, which is economically advantageous for material studies. Spherical gas atomized Ti-6Al-4V powder was used with size distribution in the range of 15–45 μm , specified as ASTM Grade 23 ELI, with chemical compositions of <0.13% O, <0.03% N, <0.08% C, <0.25% Fe, <0.01% H, Y<0.01%, supplied by Renishaw Inc. The powder bed was not pre-heated and was purged with argon to keep the oxygen level below 100ppm. The dimensions of the cuboids were $45 \times 10.8 \times 10 \text{ mm}$, with the latter dimension being the height (length in the BD). Two of the cuboids and their dimensions can be seen in Figure 41.

In order to induce different amounts of intrinsic heating while keeping a negligible porosity, a baseline of optimised process parameters was slightly modified for each build. These modifications included changes in the hatch spacing or rescanning each layer several times with different laser power, which is expected to increase intrinsic heating without significantly affecting the melt pool and therefore the porosity [150]. Furthermore, two blocks were also heat treated to study how the developed framework can be used to predict the effect of heat treatments. The baseline optimised parameters are provided in Table 5. Figure 39 shows schematics of popular scan strategies, which can be helpful to understand the different strategies used throughout the thesis. The process parameters used for each cuboid are explained in Table 6. Some cuboids were manufactured in the same print, which is important to note because it affects the time it takes to scan between each layer, influencing the thermal history. The different cuboids have been named with C#, and what build they belonged to with B#. C1 was printed by itself in the first build B1, C2 and C3 were printed together in a second build B2 and C4 and C5 were printed together in the last build B3. HT#### refers to the two different applied heat treatments, with the number being the holding temperature. The heat treatments were performed in a vacuum furnace for 2 hours and then slowly furnace-cooled for 24 hours with a cooling rate of approximately 0.07°C/s . Figure 40 includes a picture of two of the cuboids that were manufactured in the same build.

Table 5. Baseline process parameters used for the in-house powder-bed AM samples made for experimental validation.

Baseline Process Parameters	
Scan Speed (v)	1153 mm/s
Laser Power (Q)	320 W
Laser Spot Radius (r)	37.5 μm
Layer thickness (t_{layer})	60 μm
Platform Temperature (T_{preheat})	26 $^{\circ}\text{C}$
Hatch Spacing (h)	95 μm
Recoater time	12 s
Focal Offset Distance (FOD)	0 mm
Scan Strategy	Meander

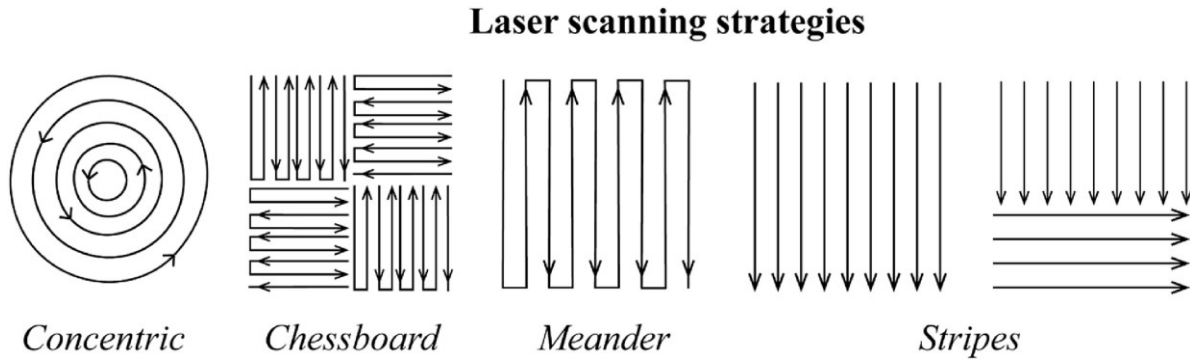


Figure 39. Schematic of popular scan strategies used in LPBF. Reproduced from ref. [151].

Table 6. Process parameters for each cuboid of the in-house built AM samples made for experimental validation. The letter C# corresponds to cuboid. The letter B# corresponds to what build the cuboids were printed on. HT### refers to the heat treatment holding temperature applied.

In-house Process Parameters for each Cuboid	
C1-B1	Baseline process parameters
C2-B2	Half hatch spacing and rescanned 1 time each layer with full power
C3-B2	Rescanned 1 time each layer with full Power
C4-B3	Rescanned 6 times each layer with $\frac{3}{4}$ of power
C5-B3	Rescanned 6 times each layer with $\frac{1}{2}$ of power
C3-HT800	C3 heat treated 800 $^{\circ}\text{C}$ 2 hours, furnace cooled
C5-HT850	C5 heat treated 850 $^{\circ}\text{C}$ 2 hours, furnace cooled

For metallographic analyses, the samples were machined using wire Electrical Discharge Machining (EDM) and prepared by conventional grinding and polishing. Metallography was performed using SEM in backscattered electron mode at 15kV accelerating voltage. Micrographs were taken close to the centre of the cuboid at 3 different heights to study microstructural heterogeneity. The positioning of the SEM micrography for each cuboid is shown in Figure 40.a). The 3 different imaging regions are referred to as top, middle and bottom in the results section with respect to their height in the building direction.

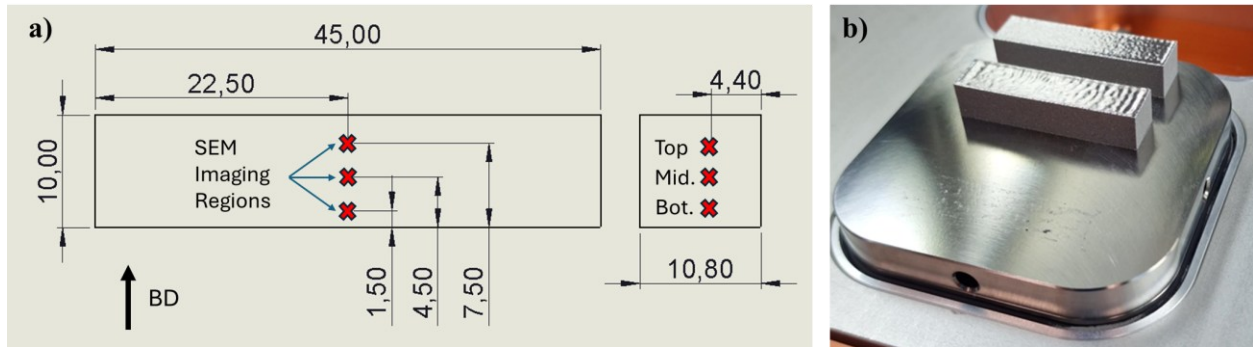


Figure 40. **a)** Drawings of the printed cuboids showing their dimensions and the positions of the SEM micrographs taken. Units are in mm. **b)** Image of two cuboids after printing on top of the build plate inside the RBV module; they correspond to C4-B3 and C5-B3.

4.2.2 Validation with data from Literature

Since the RBV set up used did not allow to pre-heat the build plate, which can influence solid-state phase transformations, the model was also validated against measurements from the literature which pre-heated the build plate. The work from Xu et. al. was used [152]. In this reference, several LPBF Ti-6Al-4V samples were manufactured with different process parameters, and their microstructures were analysed with SEM to study the effect of thermal cycles on phase transformations. They printed supported cylinders with 3 different inter-layer times and showed how this can have an impact on the microstructure and mechanical properties of Ti-6Al-4V. The process parameters used are displayed in Table 7. More information about their experimental procedure can be found in ref. [152]. Micrographs from the reference have been used for quantitative microstructural analysis to validate the developed model by simulating the process for each cylinder.

For the simulation, the microstructure evolution was modelled at the centre of the cylinders at mid height. The CAD model of the supported cylinder used in the thermal FEA model can be seen in Figure 41. The cylinders had a diameter of 12 mm and a height of 100 mm. The area fraction of the supports in contrast to cylinder cross-section was 0.4.

Table 7. Process parameters used for the 3 cylinders taken from literature for experimental validation. Each cylinder used a different recoater time.

Scan Speed (v)	1029 mm/s
Laser Power (Q)	370 W
Laser Spot Radius (r)	35 μm
Layer thickness (t_{layer})	60 μm
Platform Temperature (T_{preheat})	200 °C
Hatch Spacing (h)	120 μm
Recoater time	1, 5 and 8 s
Focal Offset Distance	2 mm
Scan Strategy	Chessboard

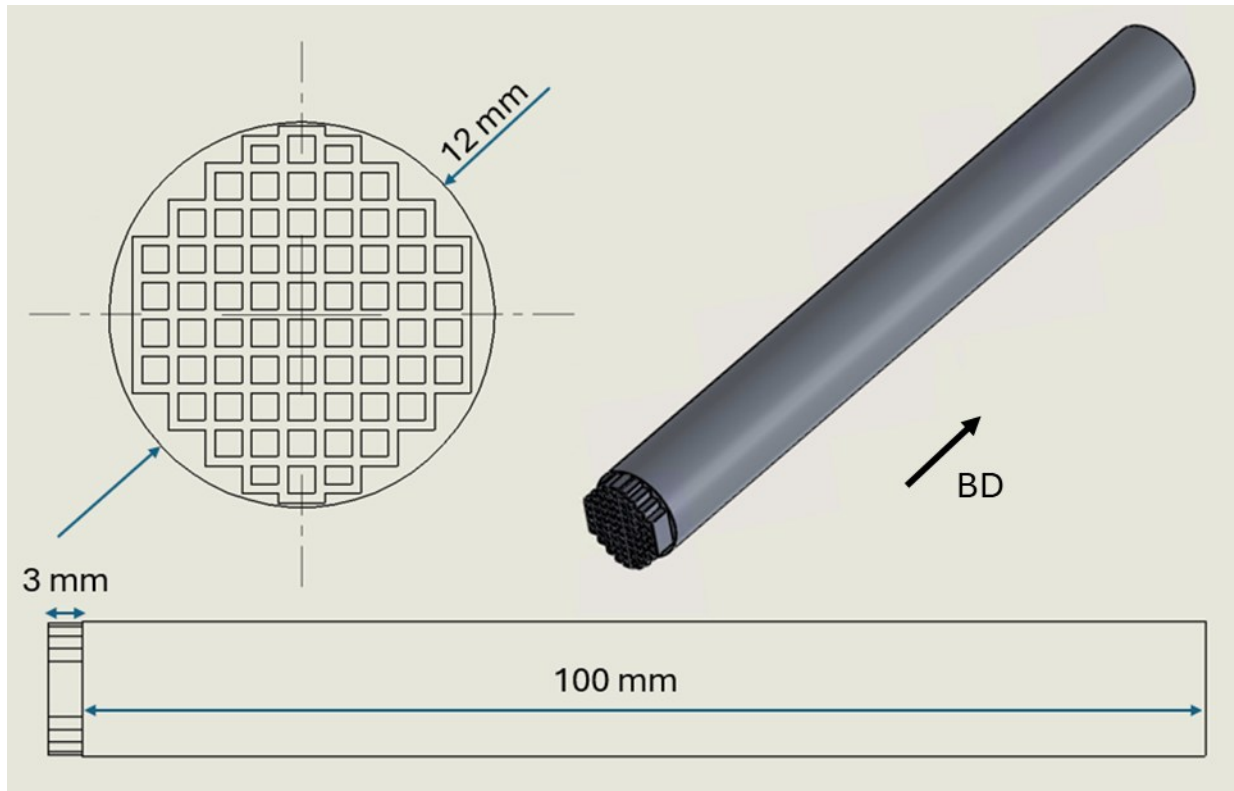


Figure 41. CAD model used in the thermal FEA model of the LPBF process of the cylinders from ref. [152].

4.2.3 Measurement of microstructural features with SEM image analysis

The image analysis was performed using the image processing software MIPAR. The micrographs used had different sizes depending on the grain sizes seen, adjusted to include enough features. The figures in the results section (Section 4.3.2) show some of these micrographs.

The BSE images used were processed with denoising, median blur, thresholding, morphological opening and removal of small objects. This pre-processing was based on the work from ref. [153]. The phase fraction of f_β was estimated as the white region in the image after applying thresholding (separate into black and white regions), with the rest of the image being f'_α or f_α . Since it is not possible to differentiate α from α' through SEM, the martensite fraction f'_α was estimated qualitatively as fully martensitic ($f'_\alpha = 100\%$) if no β was visible, partially decomposed ($f'_\alpha = 50\%$) if β was only seen at some α/α' grain boundaries (GBs) and fully decomposed ($f'_\alpha = 0\%$) if β was visible in all the α/α' GBs. Using the appearance of β is a common approach to identify the presence of α' [152]. The lath thicknesses t_α were measured manually, taking the average of 10 different laths. Using the mean inverse line intercept as suggested by ref. [153] did not work well for small laths or not fully decomposed microstructures.

This analysis was performed for three Backscatter Electron (BSE) micrographs at each analysed position of the sample. The obtained microstructural values for the three distinct micrographs were then averaged, and the maximum error was also reported calculated as $E_{max} = (x_{max} - x_{min})/2$.

4.3 Results and Discussion

4.3.1 Comparison with XRD measurements

Figure 42 shows the comparison between the predicted phase fraction and the experimental XRD measurements during the DED process from ref. [149]. Figure 42.a) shows the comparison between the total α fraction, which consists of the addition of the α' and α fractions ($f_{(\alpha+\alpha')}$), since α and α' could not be differentiated by XRD. Looking at the results, the model predicts well the kinetics of phase transformation during the recorded thermal history, with an error on the final phase fraction prediction of less than 3%. Since the model prediction is matching well with results of XRD measurements, and that the XRD did not differentiate between α' and α , the model can

be trusted to estimate the fractions of these phases. Figure 42.b) shows the breakdown of the phase fraction predictions by the model, where it is seen that the subsequent thermal cycles fully decompose the martensitic α' , which is common in DED of Ti-6Al-4V [154, 155].

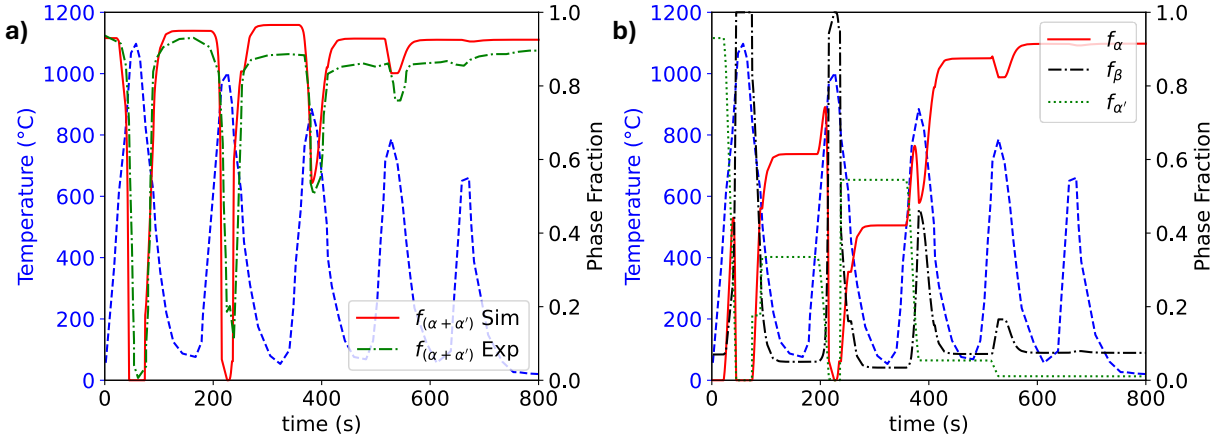


Figure 42. **a)** Comparison of the predicted microstructure evolution by the model developed in this thesis (i.e., $\alpha + \alpha'$ fraction) with in-situ XRD measurements for a DED process of Ti-6Al-4V. Experimental data extracted from ref. [82]. **b)** Breakdown of the predicted phase fractions (α' and α) by the microstructure evolution model.

4.3.2 Comparison with SEM micrographs

The following figures compare the predicted phase fraction and lath thickness by the developed microstructure evolution model with SEM micrographs taken from the in-house built samples in their as-printed conditions. The comparisons are performed along different positions of the builds with varying process parameters. Each figure shows the evolution of thermal history simulated with the thermal model, explained in **Chapter 3**, and the predicted phase fractions and lath thicknesses together with an experimental micrograph of the final microstructure. They also show a table with the microstructural predictions at the end of the process and the experimental measurements obtained from the micrographs.

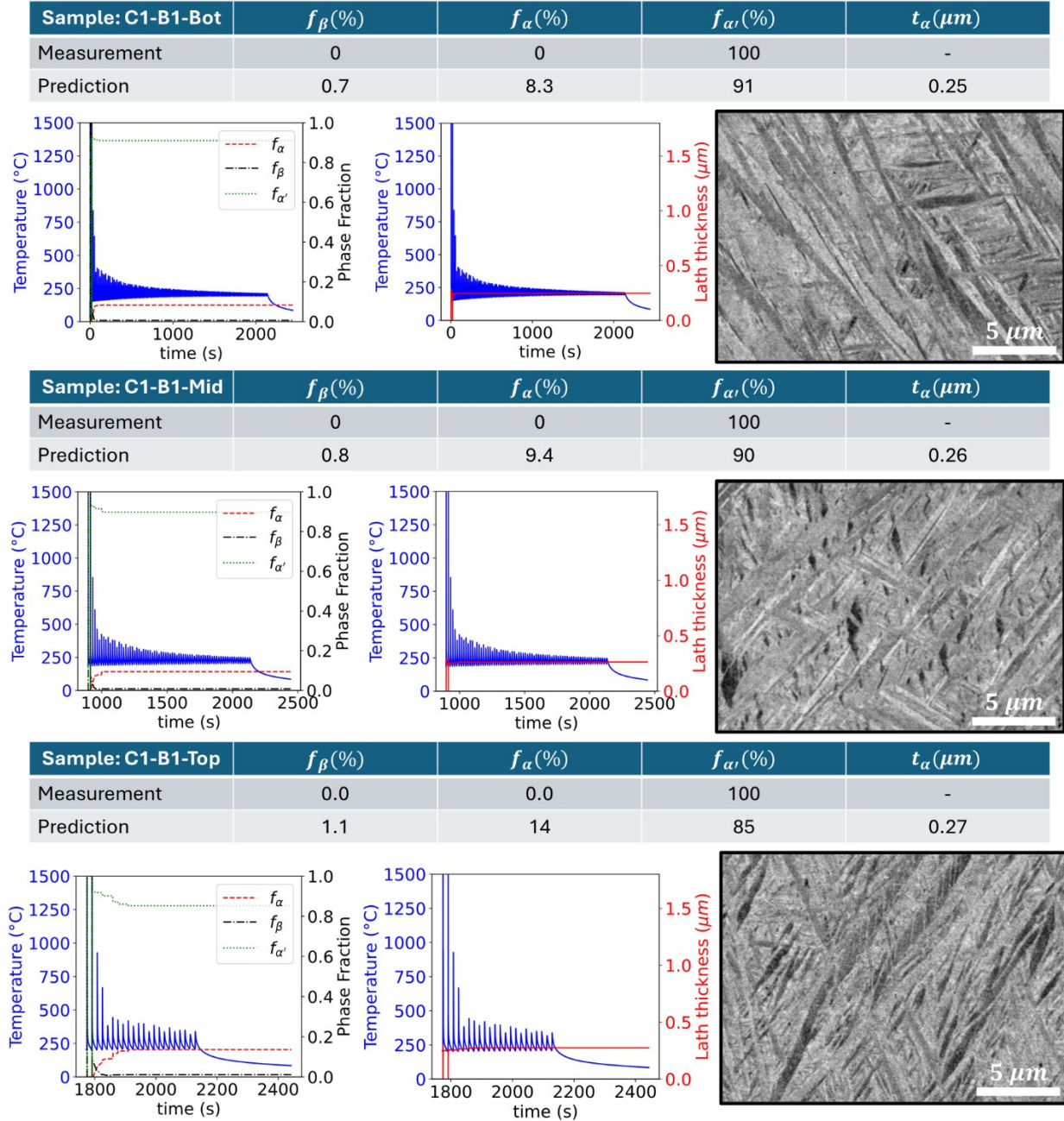


Figure 43. Microstructure Evolution Model results for sample C1-B1 and experimental measurements together with BSE image of the final microstructures. C1-B1 was manufactured with standard process parameters.

Figure 43 compares the modelling results with the experimental measurements of the as-built microstructure corresponding to sample C1-B1, which was manufactured with the baseline process parameters. The micrographs show a fully martensitic microstructure for the 3 positions in this sample, characterised by a hierarchy of thin laths with low contrast in their grain boundaries and

the presence of twins. This martensitic microstructure is expected as it is the common microstructure that appears after powder bed fusion in small components, since they do not accumulate significant heat [156]. The model correctly estimated the martensitic microstructure although showing a small quantity of β and α , which are likely to be present in the microstructure according to [152], but cannot be captured with SEM.

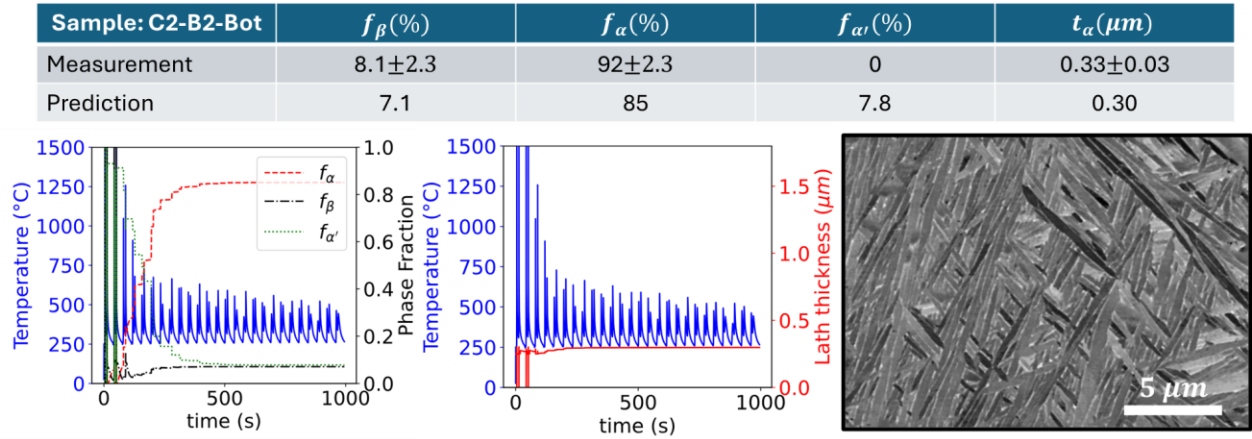


Figure 44. Microstructure Evolution Model Results for sample C2-B2 and experimental measurements. C2-B2 was manufactured with half of the standard hatch spacing and rescanning each layer once. Only one position was analysed because the print had to be stopped early due to balling up effect appearing.

Figure 44 corresponds to the results from cuboid C2-B2, whose process parameters were modified from the baseline by decreasing the hatch spacing to half and rescanning each layer twice, which increased significantly the heat accumulation. This increase in heat promoted martensite decomposition leading to a lamellar $\alpha + \beta$ microstructure, which can be easily distinguished from the martensite due to the appearance of bright β in the α lamellae boundaries. However, this increase in heat produced a balling-up effect and the build had to be stopped, only yielding one analysis region (i.e., bottom of the build). The balling-up effect is a common defect in LPBF where the molten track breaks up into a series of disconnected, spherical droplets rather than forming a continuous, smooth bead; usually due to over-heating [157, 158]. The model correctly predicted the martensite decomposition and the correct fraction of β . It also correctly estimated the α lath thickness t_{α} . However, this sample shows that a microstructure evolution model should not be the only tool used to optimise process parameters, as other detrimental effects can show up when

varying process parameters. This means that a full digital twin to optimise process parameters in AM will require several models combined together, such as one to predict microstructure and properties like the model presented in this work, but another to predict melt pool stability.

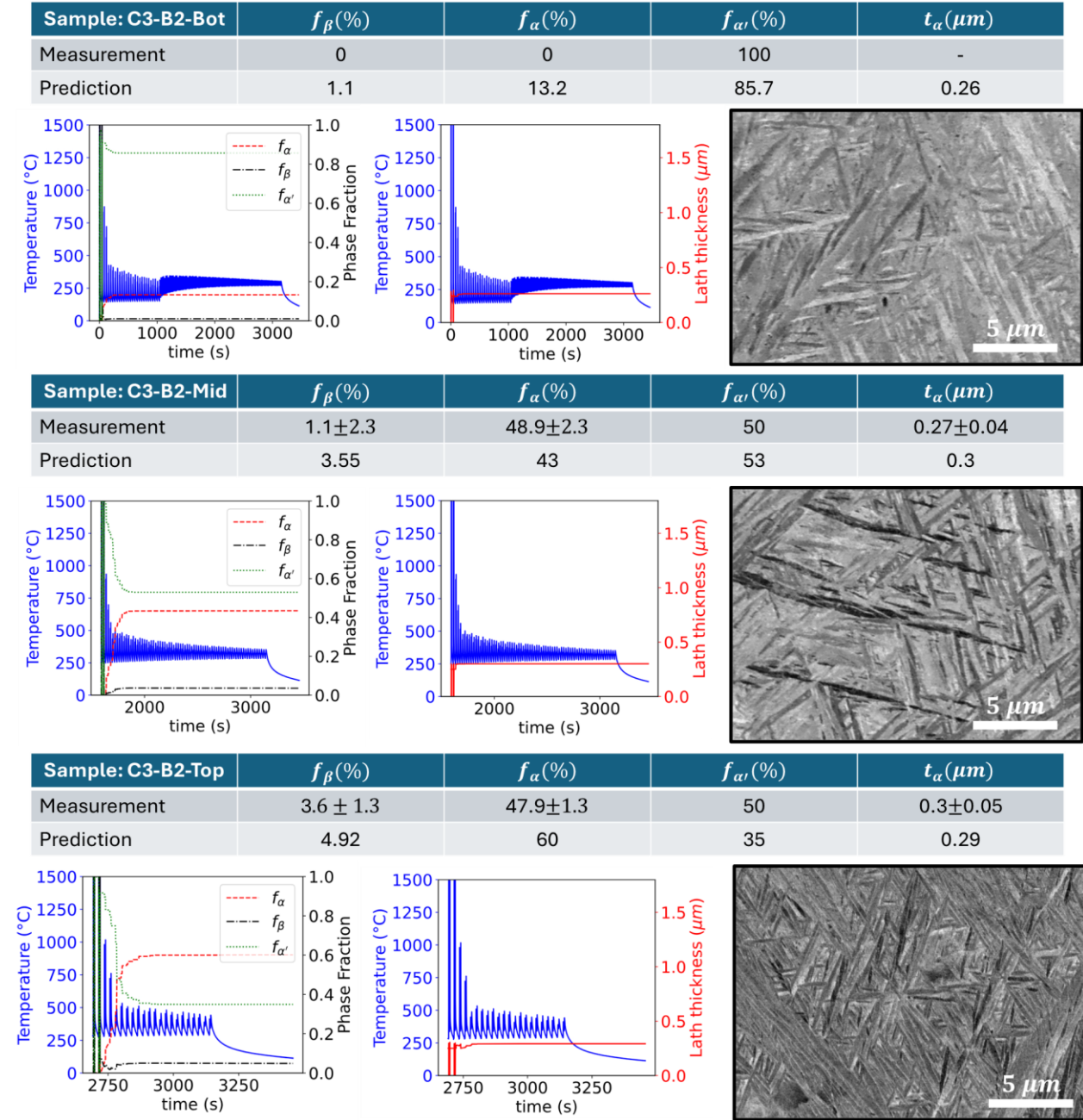
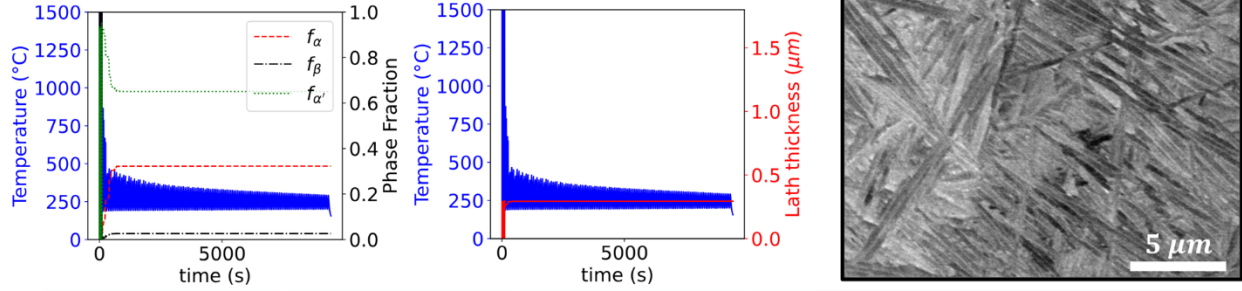


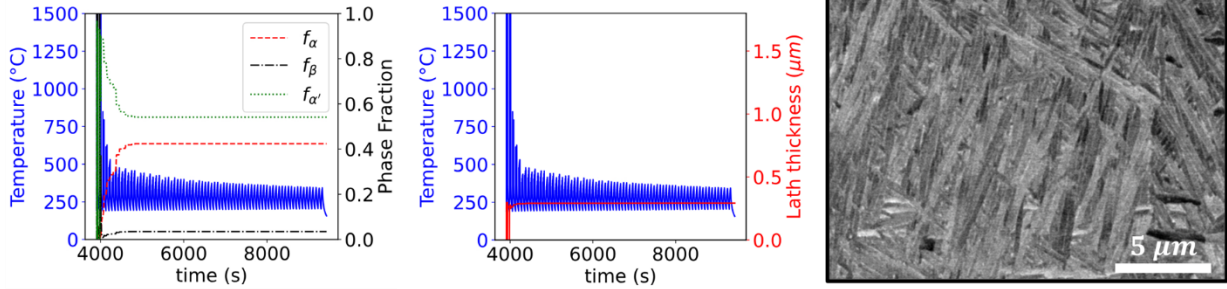
Figure 45. Microstructure Evolution Model results for sample C3-B2 and experimental measurements. C3-B2 was manufactured with the default parameters but rescanning each layer once. This sample was manufactured in the same build as C2-B2, which affected the thermal history.

Figure 45 shows the analysis for sample C3-B2, which was manufactured with the standard parameters but rescanning each layer once. Since it was printed in the same build as sample C2-B2 (presented in Figure 44), the inter-layer time decreased when the printing of C2-B2 was stopped, which increased the heat accumulation. This can be clearly seen in the thermal history for sample C3-B2-Bot, where a sharp change in heat accumulation can be seen at around one third of the printing time. This change in heat accumulation seems to have affected the microstructure, as the bottom region C3-B2-Bot shows a martensitic microstructure, while the upper regions that were printed after the reduction in inter-layer time (C3-B2-Mid and C3-B2-Top) show a partial martensite decomposition. This was correctly predicted by the model, but it seems to have overestimated the fraction of β slightly.

Sample: C4-B3-Bot	$f_{\beta}(\%)$	$f_{\alpha}(\%)$	$f_{\alpha'}(\%)$	$t_{\alpha}(\mu m)$
Measurement	2.5 ± 2.1	48 ± 2.1	50	0.30 ± 0.05
Prediction	2.7	32	65	0.29



Sample: C4-B3-Mid	$f_{\beta}(\%)$	$f_{\alpha}(\%)$	$f_{\alpha'}(\%)$	$t_{\alpha}(\mu m)$
Measurement	4.3 ± 3.1	45 ± 3.1	50	0.30 ± 0.03
Prediction	3.5	42	54	0.29



Sample: C4-B3-Top	$f_{\beta}(\%)$	$f_{\alpha}(\%)$	$f_{\alpha'}(\%)$	$t_{\alpha}(\mu m)$
Measurement	4.0 ± 2.0	46.0 ± 2.0	50	0.29 ± 0.05
Prediction	4.3	52.0	44	0.30

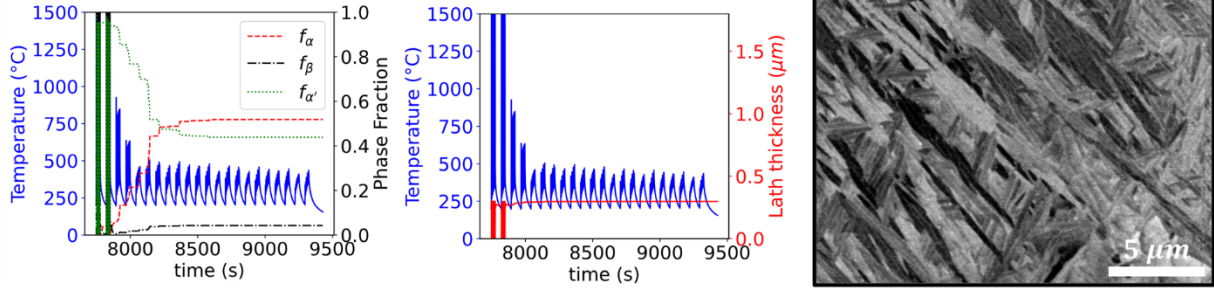


Figure 46. Microstructure Evolution Model results for sample C4-B3 and experimental measurements. This sample was manufactured with the baseline parameters but rescanning each layer 6 times with $\frac{3}{4}$ of the baseline power ($P_{rescan} = 240 \text{ W}$)

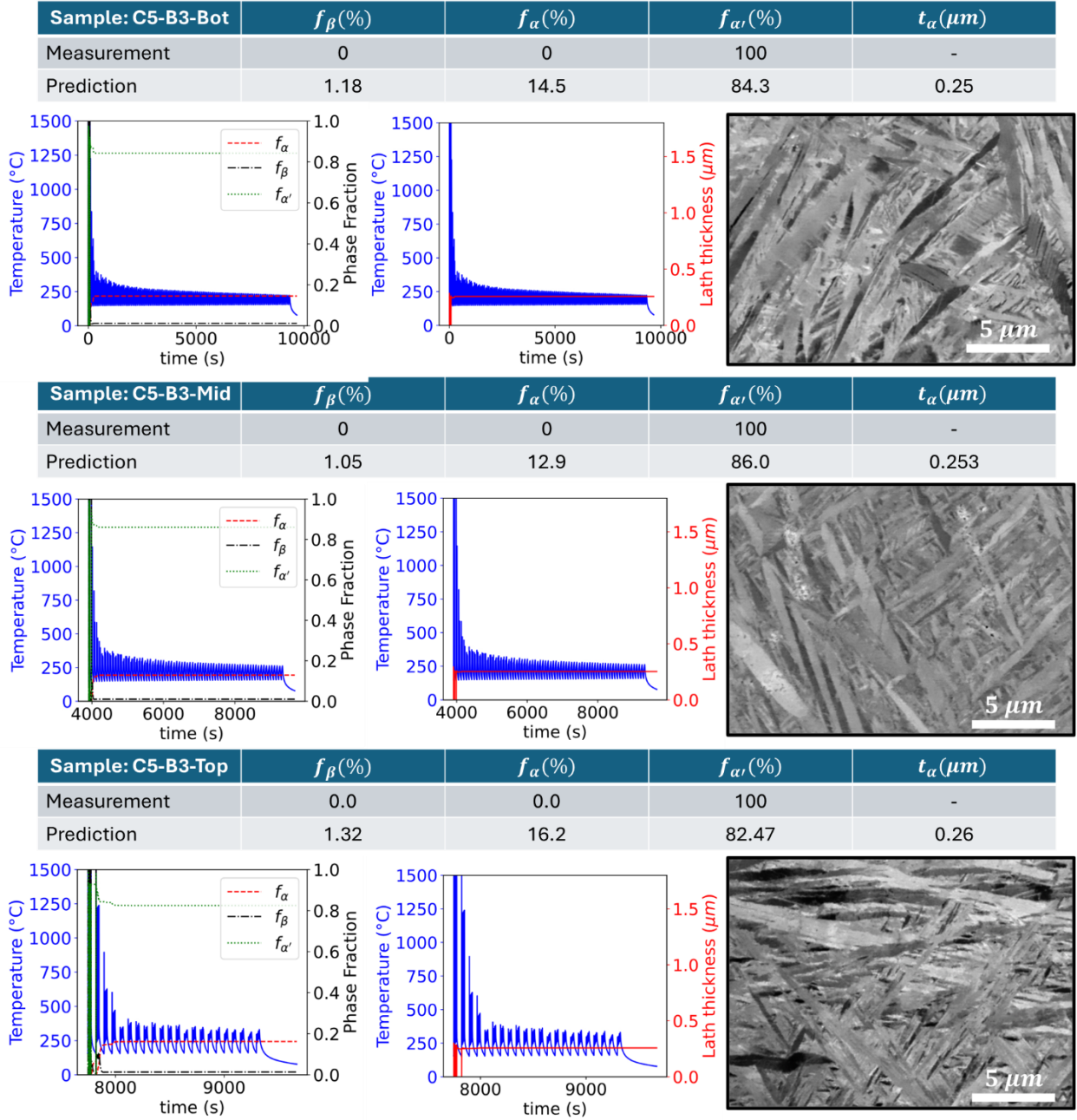


Figure 47. Microstructure Evolution Model results for sample C5-B3 and experimental measurements. This sample was manufactured with the baseline parameters but rescanning each layer 6 times with $\frac{1}{2}$ of the baseline power ($P_{rescan} = 160 \text{ W}$).

Figure 46 and Figure 47 show the results for samples C4-B3 and C5-B3, respectively. These samples were printed using the baseline parameters but rescanning each layer 6 times with different laser powers in each sample. C4-B3 was rescanned with a power corresponding to $\frac{3}{4}$ of the baseline power ($P_{rescan} = 240 \text{ W}$), while C5-B3 was rescanned with $\frac{1}{2}$ of the baseline power ($P_{rescan} =$

160 W). The difference in rescanning power affected the heat accumulation and the final microstructure. C4-B3, with a higher rescanning power ($P_{rescan} = 240\text{ W}$), shows a partial martensite decomposition, while the microstructure in C5-B3 ($P_{rescan} = 160\text{ W}$) remained fully martensitic as it did not accumulate enough heat. This difference in decomposition was predicted by the model, which also predicted well the final lamellar thickness in the partially decomposed sample (t_α).

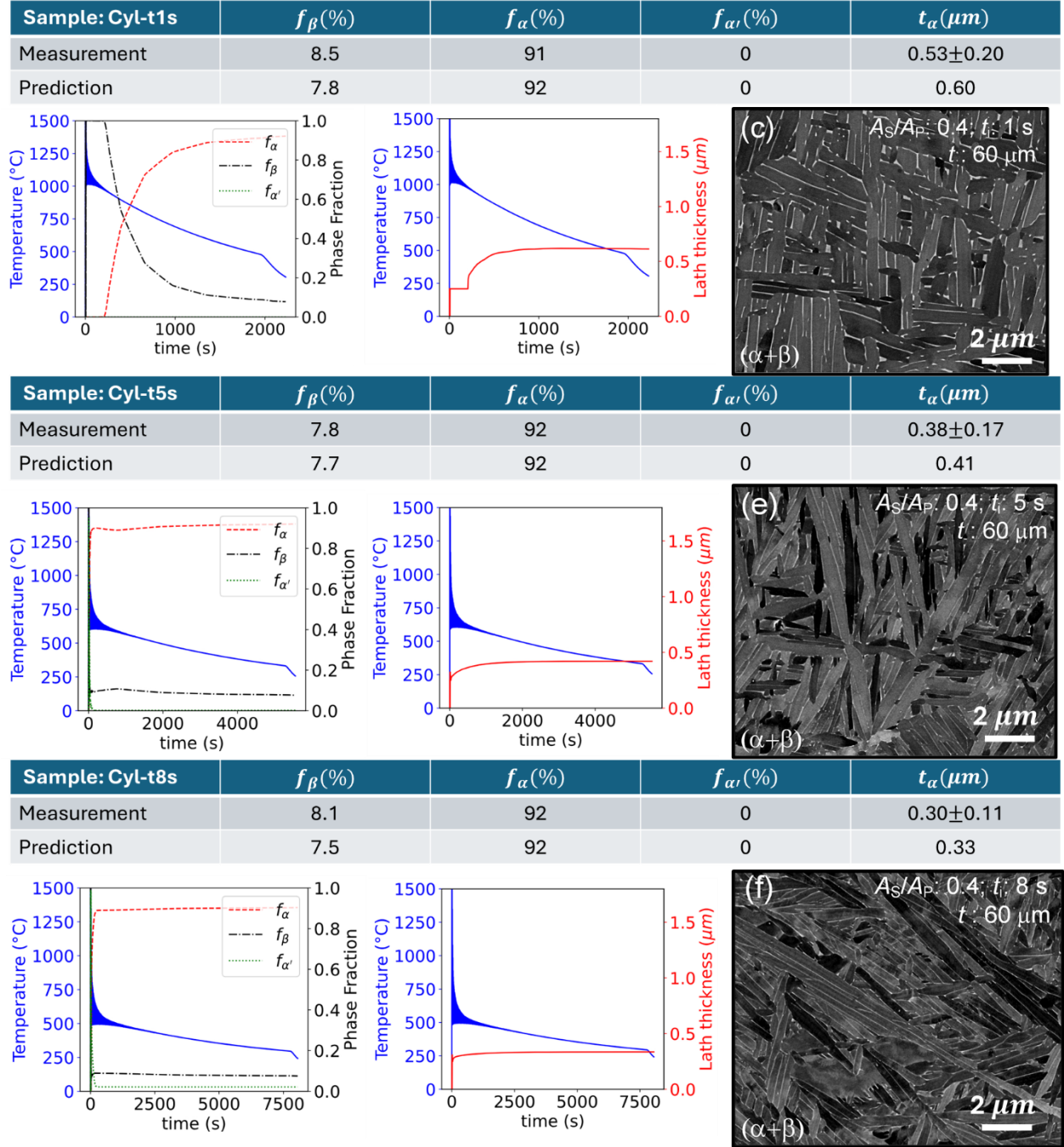


Figure 48. Microstructure Evolution Model results for the conditions taken from ref. [152]. Each of the microstructures correspond to the middle region of a different cylinder. All the cylinders were printed with the same scanning parameters but modifying the inter-layer time, which is specified in the sample name. The micrographs shown were reproduced from ref. [152].

Figure 48 shows the validation of the model using the experimental data from ref. [152]. Each micrograph corresponds to the middle region of a different cylinder. All cylinders were

manufactured using the same AM scanning parameters, but using different inter-layer times. Since these cylinders were printed using a pre-heated build plate and fairly short inter-layer times, they all contained fully $\alpha + \beta$ microstructures, as has been predicted by the model. Nonetheless, the impact of the inter-layer time produced significant differences in heat accumulation, which affected the final lath thickness (t_α). The samples with lower inter-layer time accumulated more heat and the α laths coarsened, leading to higher t_α . This effect was accurately predicted by the model, which yielded a good estimate of the final t_α .

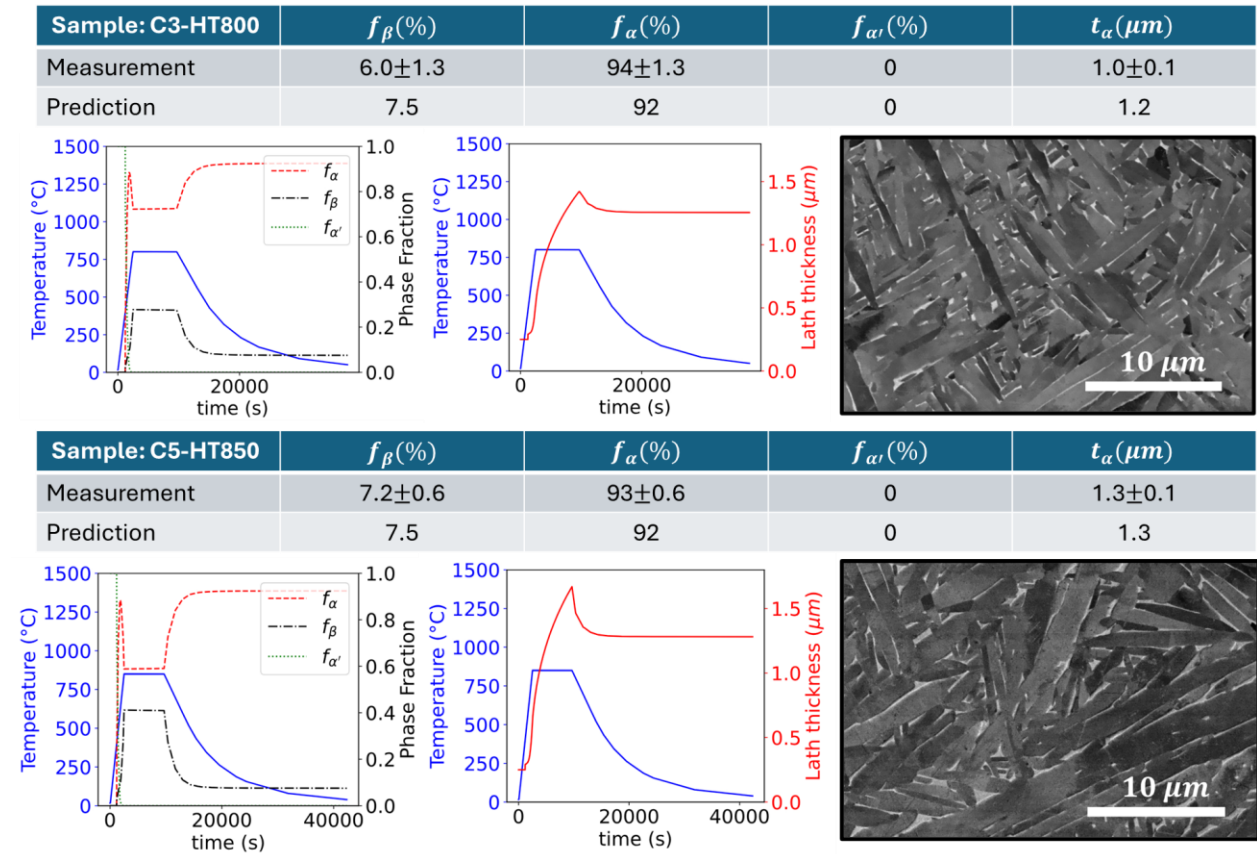


Figure 49. Experimental validation of the Microstructure Evolution Model results for the heat-treated samples. C3-HT800 corresponds to sample C3-B2 heat treated at 800 °C and C5-B3 corresponded to sample heat treated at 850 °C. Both were heat treated for 2 hours, and slow furnace cooled (~ 0.7 °C/s).

Finally, Figure 49 corresponds to the analysis of the heat treatment of two of the previously analysed samples. The temperatures used as input for the microstructure evolution model were obtained from thermocouples in the furnace. C3-HT800 corresponds to sample C3-B2 heat treated

at 800 °C and C5-HT850 corresponded to the C5-B3 sample heat treated at 850 °C. Both were heat treated for 2 hours, and slow furnace cooled at 0.7 °C/s. They both had similar microstructures after printing; therefore, the initial microstructure is not expected to affect the results posterior to the heat-treatment. For this reason, they were both initialised to a fully martensitic microstructure before the microstructure evolution simulation. Only one micrograph is included for each sample as the heat treatments homogenised the microstructure and no different in microstructure was seen along the sample.

After the heat treatments, as expected, both samples contained a fully decomposed $\alpha + \beta$ lamellar microstructure and much thicker lamellae than the as-built samples. The difference in heat treatment temperature produced a higher t_α in sample C5-HT850, due to the higher heat treatment temperature. This effect was predicted by the model, and it yielded a good estimate of the final t_α ; nonetheless, the model overestimated t_α in sample C3-HT850 and underestimated the difference in t_α between both heat treatments.

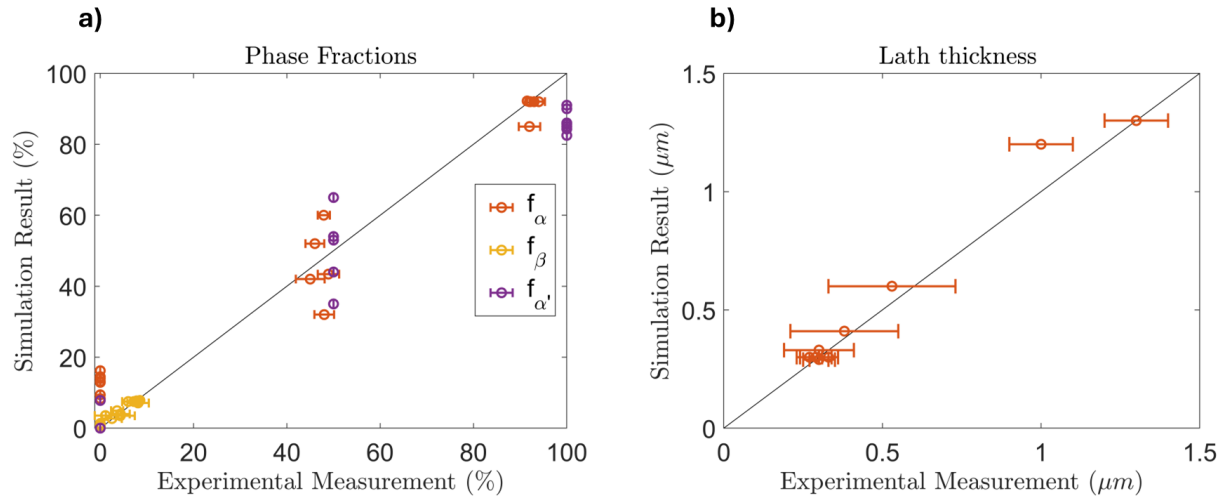


Figure 50. Comparison between the simulated and measured values for all the samples analysed with SEM. a) Simulation results against experimental measurements for the phase fractions ($f_\alpha, f_\beta, f_{\alpha'}$). b) Simulation results against experimental measurements for the lath thickness (t_α). The error bars show the maximum error calculated as $E_{max} = (x_{max} - x_{min})/2$.

To summarise, the comparison between the microstructure evolution model results and the experimental measurements have been compared in Figure 50 for all the samples analysed with SEM. In these plots, the proximity of the scattered points to the diagonal lines yields an estimate

of the accuracy. Overall, the model has yielded good estimates of the final microstructures for different geometries and process parameters, as well as heat treatments. The most notable errors were in the prediction of the α/α' phase fractions in partially decomposed samples, which are not measurable through SEM and could not be validated accurately. However, the model was able to infer if martensite decomposition started and if a fully $\alpha + \beta$ microstructure was reached, at least qualitatively. Another inaccuracy was found in the calculation of lath thickness during the heat treatments, which predicted a small difference between the two heat treatment temperatures. It is likely that a more non-linear phenomenological equation for the lath thickness evolution equation and better calibration of the phenomenological constants will be needed to correct for this. Also, part of the deviation is likely caused by carrying over the uncertainties in the thermal model, previously discussed in **Chapter 3**. Nonetheless, the model yielded reliable predictions for the different microstructural features predicted in as-built samples, whose accuracy can probably be increased further by applying specific material and machine correction factors.

4.4 Conclusions

A mean-field microstructure evolution model has been developed to estimate the evolution of the microstructural features that mostly influence strength in Ti-6Al-4V. These features are namely the phase fractions (f_{α} , f_{β} and $f_{\alpha'}$) and the α lath thickness (t_{α}). The predictive capabilities of the developed model have been analysed using experimentally measured data by XRD taken from ref. [149], as well as contrasting the modelling results with the final microstructure after the AM process using SEM analyses, which was performed on in-house built samples and taken from literature. These validations included several geometries and process parameters, as well as heat treatments.

Overall, the model has been shown to capture well the kinetics of microstructure evolution in Ti-6Al-4V during AM. Moreover, it has been shown that it can be coupled with thermal FEA models to produce process-structure models that can predict microstructure given a component's geometry and its process parameters. Therefore, this work showcases the possibility of fully digitalise AM of Ti-6Al-4V with coupled properties prediction, which would allow to tune process parameters or geometry to predict a desired microstructure and mechanical properties. In the future, if the thermal model can be accelerated, it is likely that parametric optimisation tools can

be developed using similar models that will automatically tune process parameters and geometry to homogenise or optimise the microstructure for a given structural application. However, this work also showed that this potential tool will need to be coupled with other models to ensure melt pool stability, as changing parameters to achieve a given microstructure could lead to manufacturing problems, as seen for one of the samples inspected (i.e., C2-B2).

Moreover, several deviations from the measurements were seen during the experimental validation that need to be addressed in the future. Part of the uncertainty in the results is likely derived from the thermal model used to obtain the temperature histories used as input for the microstructure evolution model, which was discussed in detail in **Chapter 3**. Additionally, the parameters used in the microstructure evolution model are also uncertain and hard to obtain for the rapid thermal changes in AM. Also, measuring the final microstructural parameters is complex in as-built AM microstructures due to fine microstructures formed. The development of more standardised methods for measuring these features, both during and after the AM process, will be essential for creating more reliable structure-property models in AM. Despite these limitations, the current model, which could also be supplemented with machine and material specific correction factors, shows strong potential for providing accurate predictions of final microstructures, making it a potentially valuable tool for guiding shop-floor process engineering decisions.

5. MICROSTRUCTURE-PROPERTY MODELLING OF ADDITIVELY MANUFACTURED Ti-6Al-4V

By combining the previously developed thermal model in **Chapter 3** and microstructure evolution model from **Chapter 4**, it is possible to predict microstructural parameters along different regions of a powder bed fused component. Then, the next step in the PSPP chain is to relate these microstructural features to the mechanical properties that are most commonly used in structural design. Namely, the aim is to calculate the anisotropic elastic and yield strength properties (E, σ_y) as a function of the previously calculated lath thicknesses and phase fractions of α , α' and β . Experimental methods are the common approach to this endeavour, but are costly and time consuming, especially for the vast combination of possible microstructures that can occur in AM of Ti-6Al-4V. Instead, a computational approach via virtual mechanical testing of 3D microstructural Representative Volume Elements (RVEs) is suggested in this thesis and explained in this chapter. This approach consists of creating synthetic RVEs tailored to specific values of phase fractions and grain sizes that can be digitally tested arbitrarily to get the desired mechanical properties through computational homogenisation.

5.1 Modelling Methodology

Computational homogenisation aims to relate microstructure with effective properties in heterogeneous materials. It assumes that the characteristic length of heterogeneities is larger than the molecular dimensions but much smaller than the length scale of a macroscopic sample. Under these conditions, macroscopic properties can be determined from the geometrical features of the microstructure and the properties of its heterogeneities [159].

In the case of computational homogenisation for the mechanical properties of polycrystals, the response to deformation of a combination of different grains need to be calculated. The main approach to achieve this is by calculating numerically a boundary value problem that solves the mechanical equilibrium PDEs. This requires the development of an RVE that accurately represents the microstructure to analyse, including its crystal orientations, and a numerical model for each phase that accurately predicts its micro-mechanical behaviour. Both of these steps are explained in detail in the following subsections.

Furthermore, since computational homogenisation is computationally expensive, a Reduced Order Modelling (ROM) approach has been developed to obtain the desired mechanical properties instantly given a set of microstructural parameters $(f_{\alpha}, f_{\beta}, f_{\alpha}, t_{\alpha})$, which consists of the regression fitting of a structure-property database generated through computational homogenisation. This is explained in Subsection 5.1.5.

5.1.1 Numerical Methods for Computational Homogenisation

As explained, computational homogenisation requires numerical modelling of a material's mechanical response, which is affected by microstructure heterogeneities, to solve a boundary value problem. For a polycrystalline materials such as Ti-6Al-4V, Crystal Plasticity (CP) is used to describe material's constitutive law. CP is a computational method that predicts deformation via slip systems considering crystallographic anisotropy to model the mechanical behaviour of polycrystalline materials at micro-scale. Recently, some models have been able to include other deformation mechanisms like twinning and phase transformations, but these have not been included in this work since they are not expected to occur under working conditions of Ti-6Al-4V in service [160]. One of the main applications of CP is the homogenisation of mechanical properties like anisotropy, strength, ductility, fatigue, etc. However, since it can capture local underlying physical phenomena along a single crystal while modelling complex polycrystal systems of several hundreds of grains, it also allows to study local phenomena such as texture evolution, strain localisation and micromechanical fields. Therefore, CP is an appropriate tool in digitally predicting mechanical properties of polycrystalline materials and it is an appropriate approach for structure-property models in AM, where strong textures and phase heterogeneities can occur along a component during the build.

The main mathematical methods to perform full-field crystal plasticity simulations are CP-FEA and CP-Fast Fourier transform (CP-FFT) methods. In these methods, each grain is represented by one or several elements having a specific constitutive behaviour dictated by the phase and orientation of the specific grain. Examples of CP-FEA and CP-FFT simulations can be seen in Figure 51.

CP-FEA is more widely used and solves the mechanical equilibrium PDEs using the classic FEA Galerkin methods. CP-FEA allows to use flexible conformal meshes on arbitrary geometries and boundary conditions, which makes it more accurate for certain problems compared to CP-FFT

[161, 162], like surface roughness analysis [163]. On the other hand, CP-FFT is a spectral numerical method that relies on the properties of the derivatives of periodic fields in Fourier Space [164]. CP-FFT requires a structured grid and periodic boundary conditions, which limits its applications, but is a much faster numerical method to solve PDEs in periodic problems. Therefore, for the purpose of computational homogenisation of macro-scale flow curves that is of interest in this thesis, which requires periodic boundary conditions, CP-FFT is proven to be a very efficient alternative [165]. This is because in FFT space the convolutional integrals that are solutions of the governing equations become a simple tensorial product, instead of requiring large matrix inversions like in the FEA method [166]. This enables CP-FFT models to scale with the number of degrees of freedom n as $n \log n$, in contrast to iterative FEA solvers which scale with $O(n^2)$. This results in a significant increase in computational speed. Knowing this and given that the objective of CP in this work is computational homogenisation with periodic boundary conditions, a CP-FFT framework has been utilised.

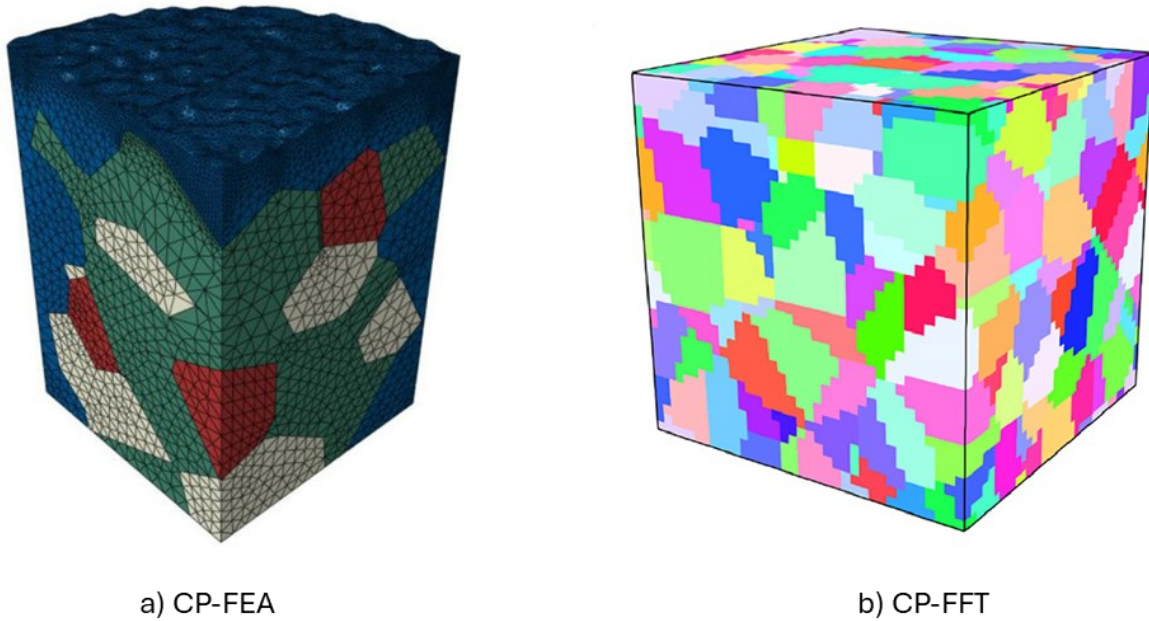


Figure 51. Examples of numerical domains for CP-FEA and CP-FFT simulations. **a)** CP-FEA simulation of surface roughness in Abaqus from ref. [167]. It shows how CP-FEA allows to use tetrahedral elements, non-periodic geometries and different mesh sizes throughout the domain. **b)** CP-FFT simulation from ref. [168], showing that a periodic geometry with a structured grid of constant voxel size is required along the domain.

Fortunately, CP simulations have started to become more accessible now. Traditionally, they have been carried out through user subroutines, like the subroutine from Huang [169], in commercial multi-purpose FEA solvers such as Abaqus. Recently, new easier to use and open-source specialised software frameworks have been developed to specifically simulate CP. For example, FEPX [170] allows to perform CP-FEM, and the grid solver in Damask [171] is a good tool to perform CP-FFT. The latter has been chosen for the CP simulations in this work.

Only an overview of Damask's grid solver approach to solve mechanical equilibrium has been presented here, more information about the spectral approach in Damask's grid solver and how these equations are solved numerically can be found in ref. [171]. This solver has been widely proven to provide fast solutions with excellent error properties [172].

CP-FFT Damask Grid Numerical Solver

The grid solver in Damask uses a spectral FFT approach to solve mechanical equilibrium by minimising the strain energy density functional $\mathcal{W}$ through iteration using Equation 17, where $P(x)$ and $P(k)$ are the first Piola-Kirchoff stress tensors in real and Fourier space, respectively:

$$\min_x \mathcal{W} \Rightarrow \text{Div } P(x) = \mathcal{F}^{-1}[P(k) ik] = 0 \quad \text{Equation 17}$$

$\mathcal{W}$ is related to the stress response through the deformation gradient F as shown in Equation 18:

$$P(x) = \frac{\delta \mathcal{W}}{\delta F}(x, F, \dots) \quad \text{Equation 18}$$

F is the total deformation gradient, and can be expressed with a spatially homogeneous part $\bar{F}$ and a locally fluctuating displacement $\tilde{F}$:

$$F = \bar{F} + \tilde{F} \quad \text{Equation 19}$$

In this way, it can be related to the deformation $\mathcal{X}(x)$ as in Equation 20, with $\tilde{w}(x)$ being the displacement fluctuation field, related to $\tilde{F}$ as $\tilde{F} = \frac{\partial \tilde{w}}{\partial x}$:

$$\mathcal{X}(x) = \bar{F}x + \tilde{w}(x) \quad \text{Equation 20}$$

Now the relationship between stress and deformation gradient needs to be established. The kinematics for elasto-plastic behaviour in Damask are defined within the finite deformation framework, where the deformation gradient is written as the product of the plastic deformation gradient F_p and the elastic deformation gradient F_e :

$$F = F_e F_p \quad \text{Equation 21}$$

The evolution of the plastic deformation gradient is calculated as in Equation 22, where L_p is the velocity gradient:

$$\dot{F}_p = L_p F_p \quad \text{Equation 22}$$

L_p is calculated from stress ($L_p = f(S, \dots)$), here the second Piola-Kirchoff stress S , through the plasticity constitutive model. The stress S is assumed to solely depend on F_e by the elastic constitutive law. In this framework, F_e is determined using the multiplicative decomposition of the total deformation gradient, calculated dynamically as $F_e = F * F_p^{-1}$. Both constitutive laws are explained in the next section.

CP Material Constitutive Model

Material constitutive models calculate the correct stress matrix S given a deformation gradient F . Firstly, the stress S is related to F_e assuming a Hookean elastic constitutive law with Equation 23, where $\mathbb{C}$ is the stiffness matrix and E the Green-Lagrange strain tensor:

$$S = \mathbb{C} : E, \quad E = \frac{1}{2}(F_e^T F_e - I) \quad \text{Equation 23}$$

Regarding the plasticity constitutive model, CP models assume that the velocity gradient L_p is composed of the summation of all the individual resolved plastic shear strain rates $\dot{\gamma}^{(i)}$ from each slip system (i). This is expressed in Equation 24, where $m^{(i)}$ and $n^{(i)}$ are the unit vectors of the slip direction and slip plane normal, respectively. The number of slip systems and the direction of these vectors at each material point will depend on the phase and crystallographic orientation of that given point.

$$L_p = \sum_i \dot{\gamma}^{(i)} * (m^{(i)} \otimes n^{(i)}) \quad \text{Equation 24}$$

Afterwards, there are several CP constitutive laws that can be used. For this work, a phenomenological CP model has been chosen. Although higher fidelity models exist like strain-gradient CP [173], these can be computationally expensive with material parameters that are hard to obtain. To calculate macroscopic flow behaviour, phenomenological CP models have proven to be reliable and are widely used [172, 174]. The constitutive model used will be described only in essence here, more details and examples can be found in [172].

In this CP model, developed by Hutchinson et. al. [175], the evolution of the shear strain in a given slip system is described by:

$$\dot{\gamma}^{(i)} = \dot{\gamma}_0 \left| \frac{\tau^{(i)}}{g^{(i)}} \right|^n \text{sgn}(\tau^{(i)}) \quad \text{Equation 25}$$

Here, $\tau^{(i)}$ represents the resolved shear stress acting on the considered slip system (i) and can be calculated from S . n and $\dot{\gamma}_0$ are the stress exponent and the reference strain rate respectively, which are phenomenological constants.

$g^{(i)}$ is the current slip resistance and it is calculated through Equation 26. Slip $\dot{\gamma}^{(i)}$ is set to occur on slip system (i) when the resolved shear stress $\tau^{(i)}$ exceeds the value of $g^{(i)}$. It evolves from the initial critical resolved shear stress τ_0 to the saturation stress τ_∞ as a function of the slip

rate $\dot{\gamma}^{(j)}$ on the other slip systems. h_0 is the initial hardening modulus and a is the strain hardening exponent, which are phenomenological constants adjusted to match the flow behaviour of the material at hand. h_{ij} is called the hardening matrix and captures the interaction between the different slip systems i and j . Therefore, this CP model is fully local and does not consider slip transmission.

$$\dot{g}^{(i)} = \sum_j \dot{\gamma}^{(j)} h_0 \left| 1 - \frac{g^{(j)}}{\tau_\infty^{(j)}} \right|^a \text{sgn} \left(1 - \frac{g^{(j)}}{\tau_\infty^{(j)}} \right) h_{ij} \quad \text{Equation 26}$$

The phenomenological CP model used is one of several CP models already integrated in Damask and can be easily chosen when setting up a model [171]. It must be noted that, as opposed to strain-gradient CP models, phenomenological CP models do not intrinsically consider grain boundary effects on local hardening. Because the physical mechanisms of dislocation pile-up and subsequent slip transmission across neighbouring grains are not explicitly modelled, the Hall-Petch effect will not be predicted even if grain geometry is captured in the RVE. In order to account for the lack of slip transmission and consider the effect of lath thickness in the structure-property model, the initial critical resolved shear stress τ_0 supplied to Damask has been set to follow Equation 27, which establishes an empirical relationship between the initial slip strength and the lath thickness through a material constant k . A Hall-Petch scaling ($\propto t_{lath}^{-1/2}$) is reasonable here because alpha lamellae make up most of the microstructure at the in-service temperatures of Ti-6Al-4V, acting as planar boundary domains that restrict the effective dislocation slip length.

$$\tau_0 = \tau_i + \frac{k}{\sqrt{t_{lath}}} \quad \text{Equation 27}$$

The explained constitutive description is applied for all the different phases modelled in this work, their micro-mechanical response is only differentiated by using different slip systems and plasticity constants. For the HCP α and α' phases, the slip systems included are the 3 basal, 3 prismatic, 6 pyramidal $\langle c \rangle$ and 12 pyramidal $\langle c+a \rangle$ families of the slip systems. However, they are differentiated by having different c/a ratios, set as 1.596 for α' and 1.604 for α . For the BCC β phase, the 12 $\{110\} \langle 111 \rangle$ and the 12 $\{112\} \langle 111 \rangle$ families of the slip systems have been

included. The calculation of the plasticity parameters for each phase is explained below in Section 5.1.3. The information regarding the constitutive properties and orientations for each grain is supplied to Damask in a text file called “material.yaml”, which is similar to a dictionary in Python such that its generation can be easily automated.

Boundary Conditions

As explained, FFT approaches require periodic boundary conditions such that only volume averaged stress or deformation values can be prescribed. For this work, only uniaxial and simple shear tensile tests parallel and perpendicular to the BD have been modelled. This is accomplished by prescribing the volume-averaged deformation gradient rate $\dot{F}$ and the first Piola–Kirchhoff stress P to target the desired stress response. Equation 28 shows the conditions applied to model a uniaxial tensile test in the X direction and Equation 29 shows the conditions for simple shear in the XY plane. $\dot{\epsilon}$ refers to the strain rate of the mechanical test and $\times$ refers to undefined components, which are free to vary throughout the simulation. In order to perform the simulation up to a desired strain ϵ , the simulation time t supplied to Damask has to be calculated with $t = \epsilon/\dot{\epsilon}$. These boundary conditions are supplied to Damask through a text file called “load.yaml”.

$$\text{Uniaxial } X \rightarrow \dot{F} = \begin{bmatrix} \dot{\epsilon} & 0 & 0 \\ 0 & \times & 0 \\ 0 & 0 & \times \end{bmatrix}, \quad P = \begin{bmatrix} \times & \times & \times \\ \times & 0 & \times \\ \times & \times & 0 \end{bmatrix} \quad \text{Equation 28}$$

$$\text{Simple Shear } XY \rightarrow \dot{F} = \begin{bmatrix} 0 & 0 & 0 \\ \dot{\epsilon} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{Equation 29}$$

5.1.2 Microstructural RVEs generation

To carry out the numerical procedures explained in the previous section, a geometrical representation that establishes the distributions of crystallographic orientations and phases in 3D space is required. This geometrical representation is then divided into a structured grid of material points where the explained numerical procedures are carried out. Each of these material points

requires a crystallographic orientation to calculate the slip system directions, and CP material parameters, which depend on the phase that the material point represents.

This section explains the method developed to generate 3D RVEs for CP simulations from the results obtained in the mean-field MEM. Although RVEs can be obtained experimentally, it is too expensive and time consuming to perform on enough microstructures to develop a PSPP model, especially in 3D. Therefore, a methodology to generate synthetic RVEs digitally and automatically is presented here.

Synthetic RVEs could be obtained from physically based full-field MEMs like Phase Field or Cellular Automaton (CA) models, but they have a high computational cost and are complex to develop in the case of Ti-6Al-4V, with no full-field models currently existing to fully model its microstructure evolution during AM. Instead, tessellation models are used which utilise geometrical and mathematical methods to represent grain morphology of a microstructure by dividing a 3D space into cells. For this work, Laguerre tessellations were used, which provide control of the size and shape of the cells and allow to accurately simulate a wide range of microstructure morphologies [176]. This approach is already a common practice, with open-software tools like Neper [177] facilitating the RVE generation process.

The main microstructures that form during AM of Ti-6Al-4V, which have been represented in the model, can be seen in Figure 52. These microstructures are formed by the appearance of α' or α lath structures inside the larger Parent β Grains (PBGs) previously formed upon solidification. The crystallographic orientations of the α/α' grains are related to the orientation of their PBGs by the Burgers Orientation Relationship (BOR). The volumetric fraction of the different phases depend on the local thermal history throughout the whole process and can vary throughout the component. However, the morphology of the PBGs is mainly columnar and homogeneous along the component, as it is determined during solidification and not usually affected by subsequent heating cycles [178]. Therefore, in this work, the morphology and texture of PBGs has been assumed constant, and only the phase fractions and grain morphologies inside them have been modified. More information about microstructure evolution and morphology can be found in the literature review, presented in Chapter 2.

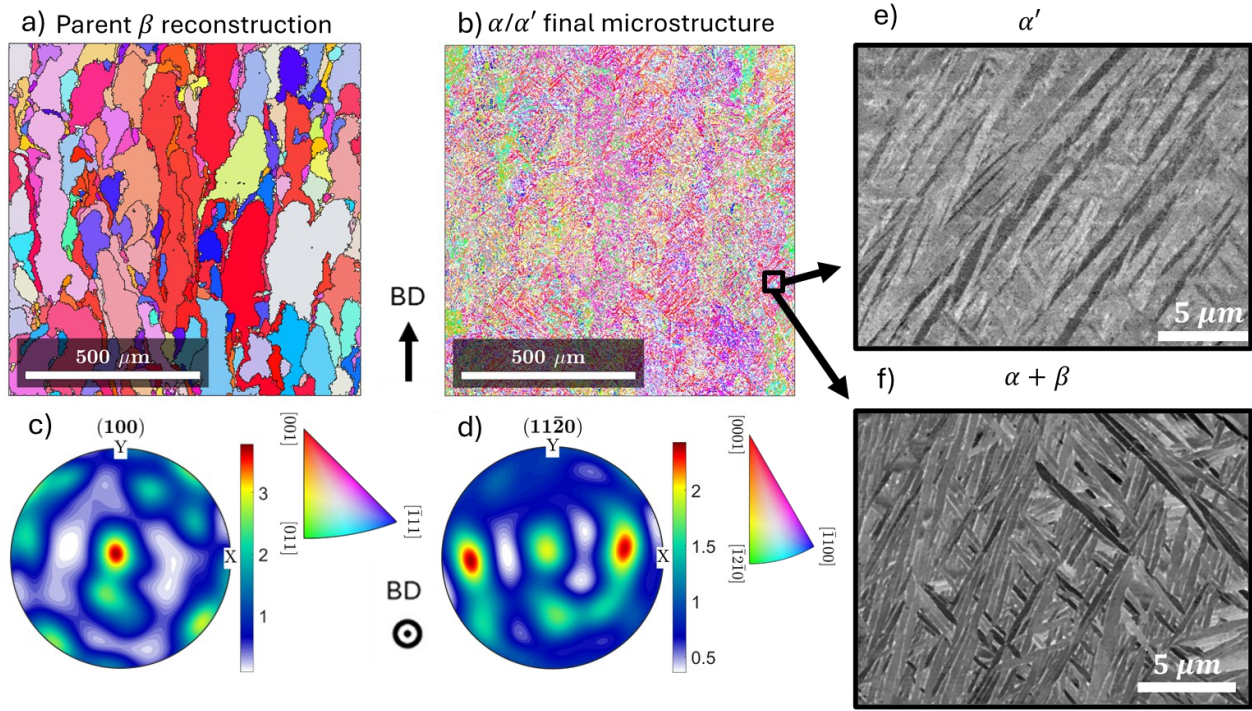


Figure 52. Scanning electron microscopy and EBSD micrographs of typical microstructures of as-built AM Ti-6Al-4V. **a)** and **b)** show the IPFs of the PBGs and real microstructure w.r.t. the Building Direction (BD), respectively. The PBGs are calculated from the real microstructure using the BOR. **c)** and **d)** show the polefigures of the PBGs and the final microstructure, respectively. The building direction is marked as BD. **e)** and **f)** show higher magnification SEM images of possible microstructures that can form inside a PBG, where **e)** corresponds to a fully martensitic microstructure and **f)** corresponds to a lamellar $\alpha + \beta$ microstructure. It must be noted that **e)** and **f)** are not the true microstructures from the EBSD in **b)**, but it is shown in this manner to explain that typical AM microstructures usually contain this PBG morphology and α/α' orientations, but with different morphology and phase fractions when analysing the lamellar morphology more closely. These final phase fractions and lath thicknesses are dependent on the thermal history experienced and are computed by the microstructure evolution model of Chapter 3.

Regarding the crystallographic orientations, the extensively studied BOR seen in Ti-6Al-4V produces local microstructural textures that need to be considered in the RVE generation, since it affects the spatial distribution of texture along the RVE and has repercussions on the mechanical properties of the alloy. The BOR in Ti-6Al-4V states that the HCP grains that form in each BCC PBG are restricted to follow the relationship:

$$\begin{aligned} (0001)_\alpha // \{101\}_\beta \\ \langle 11\bar{2}0 \rangle_\alpha // \langle 111 \rangle_\beta \end{aligned} \quad \text{Equation 30}$$

Due to the symmetries present in the cubic and hexagonal crystals, this leads to 12 possible orientations which an α grain can have from a given PBG orientation. The different possible child hexagonal orientations for a given parent cubic orientation according to the BOR are represented in Figure 53.

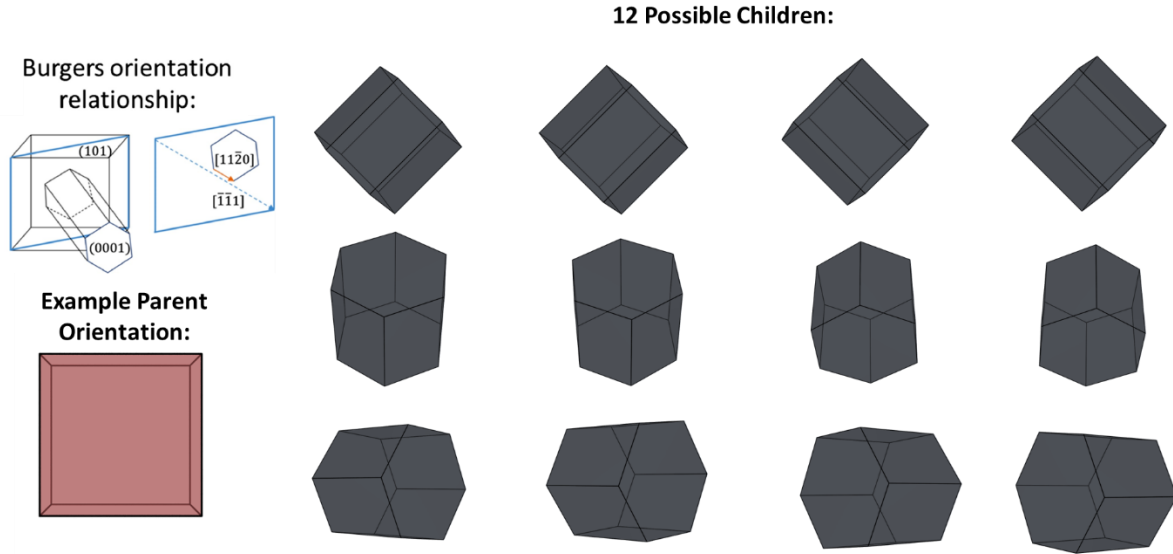


Figure 53. Representation of the BOR and the 12 possible orientations that α/α' children could have from a PBG orientation. Schematic of BOR adapted from ref. [179].

Accurate representation of these microstructures requires the use of multi-scale tessellations to model this kind of polycrystals, however, modelling the α lamellae explicitly with CP would be too computationally expensive for the case of AM Ti-6Al-4V. An example of multi-scale tessellation that was developed for trials is shown in Figure 54. This approach consists of generating α and β lamellar colonies in Neper using the cells from a bigger tessellation as domains representing the PBGs. Thereafter, orientations are assigned to the α and β lamellae based on the orientation of the PBG calculated through the BOR. More examples of multi-scale tessellations of Ti-6Al-4V for CP models can be seen in [180-183].

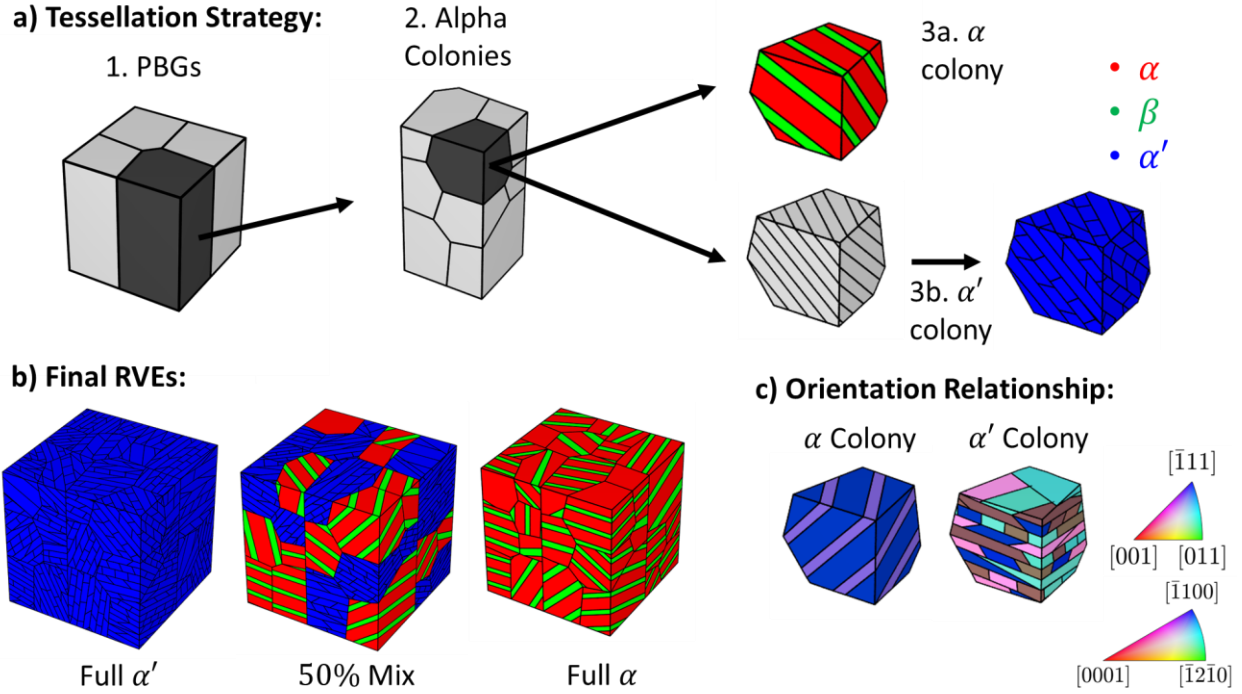


Figure 54. An example of a multi-scale tessellation procedure used to generate RVEs for AM Ti-6Al-4V. **a)** shows in different drawings how different tessellations are formed using the cell from a previous bigger tessellation as a domain to generate different colonies and lamellar structures. **b)** shows possible different RVEs depending on the phase fraction. **c)** shows the orientations and phases of the final possible α colonies. This approach has not been used for the final model because it would be too computationally expensive to model enough PBGs.

However, this approach was rejected for this structure-property model because the length-scale difference between the PBGs and the grains formed inside them is vast in AM, as shown in Figure 52. If the lamellar morphology was to be modelled explicitly, it would be too computationally expensive to include enough PBGs to obtain a representative texture in the RVE. This is caused by the large number of material points that would require the geometrical representation and orientation information of the laths.

Therefore, a simplified approach has been followed for the structure-property model in this work, where only the PBGs are represented using a Laguerre tessellation generated in Neper, and the lath structure geometry is not modelled explicitly. In this approach, after the PBG tessellation is discretised into material points (voxels), each point is assigned randomly an orientation that respects the BOR with its PBG, and a random phase while maintaining the specified phase global fractions in the RVE. Representing grains using a single material point is a common procedure

and has been proven acceptable for the purpose of computational homogenisation of macro-scale flow curves [184-188]. The consensus is that in phenomenological CP models, the texture, CP parameters and phase fractions have the main influence on the macroscopic stress-strain curves, with RVE morphology mostly affecting the microscopic response (stress distribution along the RVE) [188]. However, it must be noted that with this approach, it is not possible to get the correct stress distribution across grains, which would be required for accurate determination of material's response to fatigue or other damage mechanisms.

A summary of the RVE generation approach developed in this study is shown in Figure 55. Firstly, a periodic and columnar tessellation is generated with Neper, which is discretised into a structured grid with the desired number of material points as shown in Figure 55.a). Then, to obtain the desired phase fractions in the RVE, phases are randomly assigned to the material points inside a PBG while keeping a specific ratio to obtain the phase fractions wanted in the overall RVE. For example, if a grain has a 100 material points, and the RVE phase fraction specified is 20% β and 80% α , 20 random material points will be assigned with β material parameters, and the rest will the parameters for the α phase. An RVE with 85 PBGs and a $32 \times 32 \times 32$ grid has been chosen based on convergence studies, which showed that this high number of grains made the obtained flow curves independent of the randomness in assigned phases and texture.

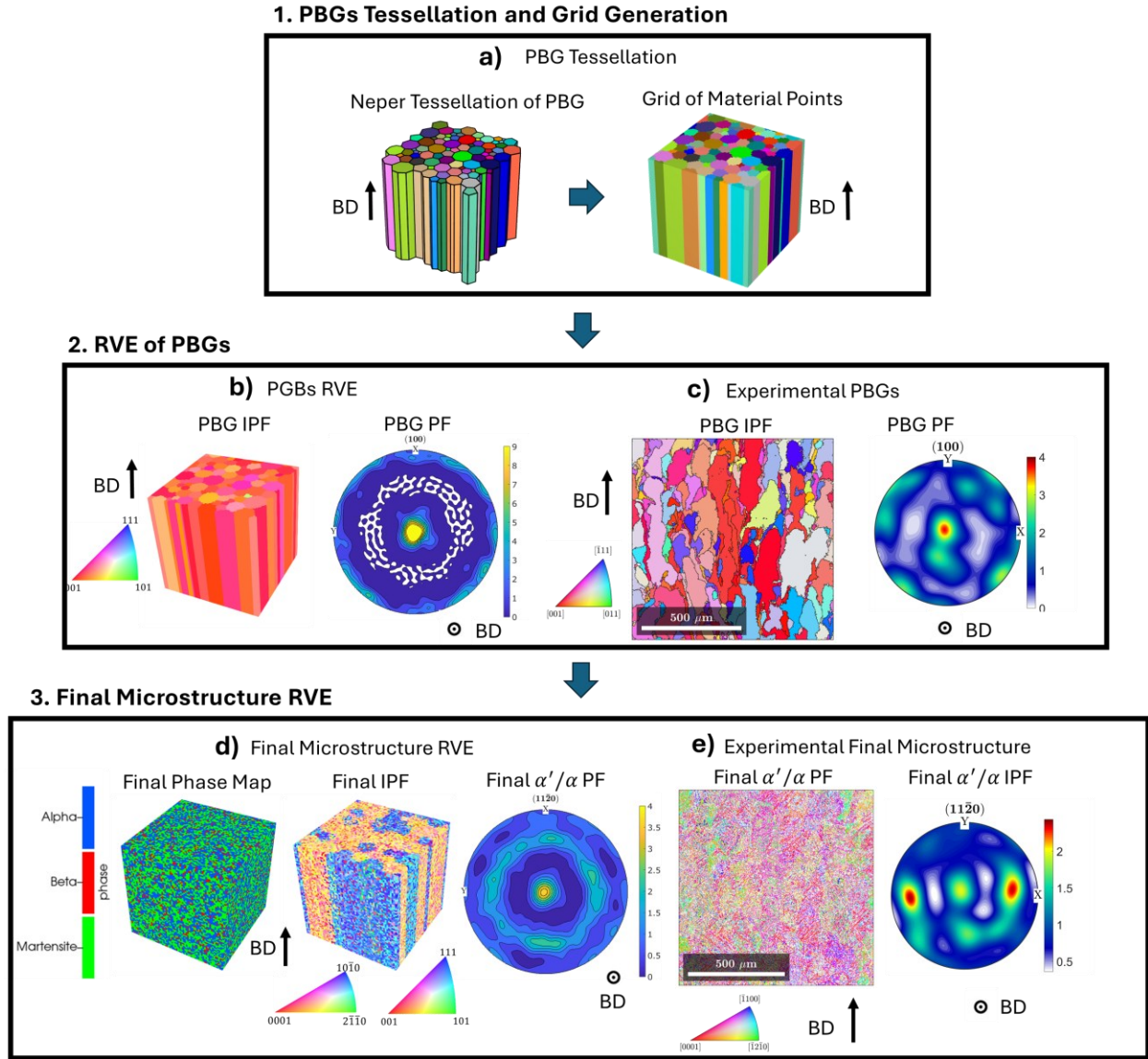


Figure 55. RVE generation procedure for the AM microstructure of Ti-6Al-4V as a function of phase fractions. **a)** Periodic columnar tessellation generated in Neper containing 85 PBGs and its discretisation in a $64 \times 64 \times 64$ grid of material points. **b)** IPF w.r.t. BD and PF of the RVE of PBGs showing their $\langle 001 \rangle_\beta$ fiber texture in the BD. **c)** Experimental counterpart of **b)** for comparison. **d)** Phase map showing the phase of each material point in an example RVE, IPF w.r.t. BD and PF of the RVE of the final microstructure. This example RVE contains 45% α , 45% α' and 10% β . The PF is shown only for the α and α' phases. **e)** Experimental counterpart of **d)**, but only the α and α' phases are shown.

Regarding crystallographic orientations, using the BOR, the orientation of each material point in the RVE can be calculated based on the orientation of its PBG. This enables the determination of the orientation of each point if the orientation of its PBG is known. One way of

obtaining the PBG texture would be a CA simulation during solidification. However, a constant PBG texture along the AM component has been assumed here, which is reasonable based on what is reported in the literature [178]. A simulation approach to obtain the PBGs texture using CA is proposed as future work.

In the current work, the PBGs have been assumed to follow a strong $\langle 001 \rangle_\beta$ fiber texture with respect to the BD, matching the PBG texture seen in the samples printed in-house through EBSD, which is also the texture commonly reported in the literature [38]. This texture is formed by the high thermal gradient in the BD, which promotes faster growth of the grains whose one of the $\langle 001 \rangle_\beta$ directions is aligned with the gradient. The texture in the RVE has been generated digitally by setting a normal random misorientation distribution of 10° between the BD and the $\langle 001 \rangle_\beta$ axis of the PBGs using MTEX [189], which is then sampled for each PBG in the RVE. The generated texture of the PBGs is shown in Figure 55.b), which matches with the experimental measurements in Figure 55.c). A synthetic texture has been used for the model because it is more statistically representative than if the ODF from the experimental EBSD was sampled, since it only contains a small region.

Then, the crystallographic orientation of the grid points inside a given PBG is calculated based on their phase. For the β phase material points, the orientation will be the same as its PBG. For the α/α' points, one of the 12 possible orientations given by the BOR with respect to its PBG will be randomly chosen. It must be noted that no variant selection is assumed in this approach, which has been reported to occur in AM, but it should not affect the final RVE texture significantly for 85 PBGs [190]. With this approach, the phases and orientations in the final RVE can be seen in Figure 55.d), which matches well with the measurements in Figure 55.e). The crystallographic orientation calculations have been implemented using MTEX [191], which allows to easily perform orientation relationship and fibre texture calculations for many grains.

The final generated RVE is supplied to Damask with the “grid.vti” and “material.yaml” files. “grid.vti” consists of a grid of numbers, where each number refers to a material in the “material.yaml” file. In “material.yaml”, each number is assigned a phase and an orientation, allowing to distribute the constitutive behaviour geometrically in the simulation and represent a polycrystal.

This RVE generation framework has been automated in a Python script that creates an RVE for the phase fractions specified and produces all the files needed by Damask to run a CP

simulation. Then, with this approach, it is possible to generate RVEs as a function of the phase fractions obtained in the microstructure evolution model of Chapter 4. However, since the geometry of the lamellae is not explicitly modelled, it is not possible to include the effect of the lath thickness in the RVE generation. This is instead considered in the CP parameters through the Hall-Petch relationship as has been explained in the constitutive model in Section 5.1.1.

5.1.3 CP Parameter Estimation

The next step in the structure-property model is to obtain the elasto-plastic material parameters for each phase. The elastic constants of a given crystal structure can usually be calculated through Ab initio methods [192] or determined experimentally [193]. Nonetheless, the required CP parameters to be implemented in the constitutive model (i.e., described in Section 5.1.1) are more intricate to calculate and are usually obtained by calibrating them to match experimental stress-strain curves. The common practice is to fit the volume-averaged stress-strain curve obtained in the CP simulation to an experimental tensile test of a microstructure with the same morphology and phases [188, 194].

For this work, there are three different phases (α , α' and β) and therefore three set of parameters to calibrate. Since calibrating all the CP parameters for the three phases at once would be too complex, two different tensile tests from ref. [195] were employed for the calibration, shown in the experimental curves of Figure 56. One of them is from an as-built sample, containing a fully martensitic α' microstructure, while the other is from a sub- β -transus heat treated sample showing a lamellar ($\alpha + \beta$) microstructure with 12% β . By separating the phases, the calibration becomes more straightforward. This way, the as-built sample can be used to calibrate the CP parameters of the α' phase in an RVE with a fully martensitic RVE, while the heat-treated specimen can be used to calibrate the α and β phases using an RVE with 88% α and 12% β , matching what was measured in the samples through SEM. As the samples were loaded parallel to the build direction, the same loading direction was applied in the CP simulations for the calibration.

Regarding the specific calibration strategy for each parameter, the elastic constants were initially obtained from the literature and calibrated to better match the elastic part of the stress-strain curve. The initial elastic constants for α' were obtained from reference [196] and for α and β from reference [197].

Some of the CP parameters were obtained from literature. γ_0 was set according to ref. [37] and a from [198], therefore using only h_0 to calibrate the hardening in this work. The latent hardening matrix h_{ij} was set to unity for the HCP phases α' and α following the assumptions made in [198-200], which imply that h_{ij} is hard to measure and the overall implication in macroscopic response is limited as the individual contributions tend to average out. For BCC β , the diagonal terms were set to 1 and the off-diagonal were set to 1.4 following the work in [201]. The rest of the parameters were all calibrated to match the plastic part of the experimental stress-strain. For the BCC β phase, the same hardening parameters are applied to all slip systems. For the HCP α and α' phases, different τ_0 and τ_∞ are applied to each slip system. In order to calibrate these, initial values for each parameter in the different slip systems were chosen based on literature values from [195] and [179], which were measured using high-energy X-ray diffraction. Then, these initial values were calibrated to match the plastic part of the experimental flow curves. The Hall-Petch constants k were initially obtained from [179], which were calibrated for Ti-6Al-4V using XRD, and then modified to match in-house experimental tensile tests with different t_α but keeping the same ratio between α and β . Once τ_0 and k are known, τ_i can be calculated with Equation 27 by measuring the lath thickness in the samples with SEM, which was $t_{\alpha'} = 0.22 \mu m$ for the fully α' specimen and $t_\alpha = 1.42 \mu m$ for the $\alpha + \beta$ specimen.

Since doing a manual calibration of all of these parameters can be cumbersome, an automatic calibration tool with an inverse optimisation algorithm was developed by combining Damask with MATLAB's surrogate optimisation solver *surrogateopt()* [202]. The developed tool automatically performs tensile test CP simulations and estimates the parameters that minimise the difference between the simulated and experimental stress-strain curves. Namely, it is minimising the cost function $f(P)$ displayed in Equation 31 [179], where P is the set of CP parameters to optimise and N is the number of points in the flow curves. σ_{sim}^i and σ_{exp}^i are the simulated and experimental stress values at the same strain for a given point, respectively. *surrogateopt()* optimisation approach works by developing a machine learning surrogate model of the relationship between the CP parameters and the cost function to minimise, and more information can be found in [202]. This allows to decrease the amount of CP simulations needed to find the optimal parameters as opposed to iterative optimisation approaches like the line search methods. A link to the code developed for the calibration tool can be found in Appendix A.3.

$$f(P) = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(1 - \frac{\sigma_{sim}^i(P)}{\sigma_{exp}^i} \right)^2} \quad \text{Equation 31}$$

Using the methodology described above, the required CP parameters were obtained for each phase; these are summarised in Table 8. The comparison between the simulated and experimental tensile curves after calibration are shown in Figure 56.

Table 8. CP parameters for each phase used in the structure-property numerical model, calibrated using the described procedure to match experimental uniaxial stress-strain curves.

Parameter	α'		α		β	Procedure
C_{11} (GPa)	150.4		168.4		137.1	Initial values were taken from literature and then calibrated to match elastic region with the same ratios
C_{12} (GPa)	82.0		94.0		98.1	
C_{44} (GPa)	43.7		49.7		48.3	
C_{13} (GPa)	58.0		67.5		-	
C_{33} (GPa)	162.7		177.7		-	
$\dot{\gamma}_0$	0.001		0.001		0.023	Literature
n	23.2		24.2		24.2	Calibrated
a	2.0		2.0		2.0	Literature
τ_i (MPa)	Basal	451.8	Basal	374.2	499.2	Initial values were taken from literature and then calibrated
	Prism	592.3	Prism	363.4		
	Pyr-<a>	600.0	Pyr-<a>	385.1		
	Pyr-<c+a>	723.1s	Pyr-<c+a>	389.5		
τ_∞ (MPa)	Basal	920.0	Basal	760.0	900.0	Initial values were taken from literature and then calibrated
	Prism	853.4	Prism	822.5		
	Pyr-<a>	941.0	Pyr-1	835.0		
	Pyr-<c+a>	113.3	Pyr-2	847.5		
h_0 (MPa)	980		1572		1200	Calibrated
h_{ij}	1		1		1 diagonal ($i = j$) 1.4 nondiagonal	Literature
k (MPa * $\sqrt{\mu m}$)	1		57.0		75.8	Initial ratio was taken from literature and then calibrated

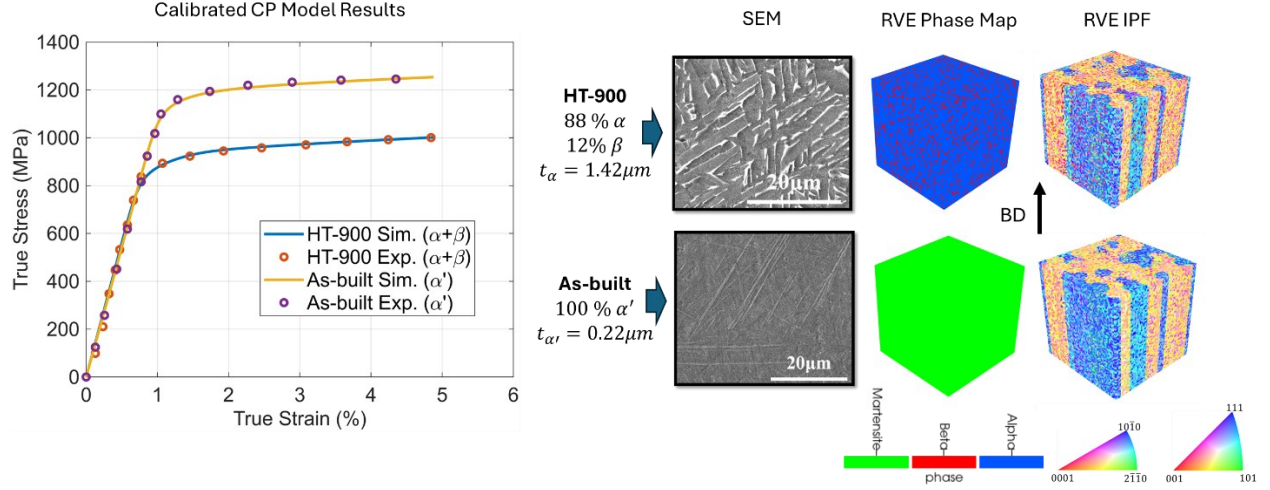


Figure 56. Comparison between the fitted and experimental stress-strain curves for the two AM Ti-6Al-4V samples used for the calibration of the CP parameters. The figure also shows the SEM images of the two samples from which microstructural features were experimentally quantified, as well as the RVEs used for the CP simulations. An as-built sample containing full α' and a heat-treated sample containing 88% α and 12% β were used for the calibrations. The phase maps and IPFs w.r.t. the BD of the RVE for each sample are shown. The SEM images and stress-strain curves were taken from [195].

5.1.4 Calculation of Effective Macro-Scale Properties from the CP Model

The objective of this chapter is to obtain a structure-property model that yields macro-scale elastoplastic properties as a function of phase fractions and lath thicknesses such that they can be used in component-scale FEA models. This has been accomplished by extracting the needed data from the simulated stress-strain curves obtained through the CP model discussed above, which is explained in this section.

After running a CP simulation of a tensile test in the desired direction using the previously explained procedures, the true stress-strain curves can be obtained by simply averaging the needed true stress and true strain components of all the material points in the RVE. In this work, the Cauchy stress tensor and the Seth-Hill strain tensor of order 0 were used as the true stress and true strain matrices.

After stress-strain curves in different directions are obtained, it is possible to calculate macro-scale effective properties from them as it would be done from experimental tensile tests. In this work, the orthotropic elastic stiffness matrix and the parameters for Hill-48 plasticity have

been calculated. Although more advanced yield criterion such as the Yld2004-18p by Barlat et. al. could be calculated to better represent the yield surface of Ti-6Al-4V made by AM [180], they require significantly larger number of tensile tests to calculate all coefficients and is proposed to be studied in future work. Nonetheless, the developed methodology would still apply for a different yield curve, as CP models allow to easily simulate an arbitrary number of tensile tests with different stress states.

Hill's potential function is a simple extension of the von Mises function, where the equivalent stress $\varphi(\sigma)$ is defined in Equation 32 as a function of the components of the Cauchy stress tensor σ . This formulation implies that yielding occurs when the equivalent stress equals to one ($\varphi(\sigma) = 1$), which corresponds to the yield curve.

$$\varphi(\sigma) = \sqrt{F(\sigma_Y - \sigma_{BD})^2 + G(\sigma_{BD} - \sigma_{XX})^2 + H(\sigma_X - \sigma_Y)^2 + 2L\sigma_{YBD}^2 + 2M\sigma_{XBD}^2 + 2N\sigma_{XY}^2} \quad \text{Equation 32}$$

F, G, H, L, M and N are the 8 material parameters that define the yield function. In this study, transverse isotropy in the plane perpendicular to the BD has been assumed, which is reasonable based on both the fibre texture and columnar morphology w.r.t. the BD of the AM microstructures [180]. However, it may be more accurate to consider both in-plane directions, and it is suggested for industrial applications. This assumption produces two symmetry conditions ($F = G, L = M$) and therefore leads to 4 parameters, which need to be calculated from 4 tensile tests. F and H can be calculated according to Equation 33, where σ_{BD}^y is the nominal yield stress in the vertical BD and σ_X^y is its analogies in for the horizontal direction. Therefore, these two parameters can be calculated with two uniaxial tensile tests perpendicular to one another (i.e., parallel and perpendicular to the BD).

$$F = \frac{1}{2(\sigma_{BD}^y)^2}, \quad H = \frac{1}{2(\sigma_X^y)^2} \quad \text{Equation 33}$$

Regarding L and N , they can be calculated with Equation 34, where σ_{XBD}^y and σ_{XY}^y are the shear yield stresses in the two planes of anisotropy. These parameters can then be obtained by two shear tests in perpendicular directions.

$$L = \frac{1}{2(\sigma_{XBD}^y)^2}, \quad N = \frac{1}{2(\sigma_{XY}^y)^2} \quad \text{Equation 34}$$

The necessary yield stresses were calculated by the common procedure of offsetting linearly fitted elastic part of the stress-strain curves and finding the intersection with the curves. As the simulated stress-strain curves have low noise, a small offset of 0.0005% strain was used to calculate the yield point. Using a small offset increases the fidelity of the plastic behaviour when it is used in macro-scale FEA models. The procedure to calculate the yield strength using an offset of the linear elastic region can be seen in Figure 57.a).

Regarding hardening, most FEA software such as Abaqus do not currently offer plasticity models with anisotropic hardening, therefore hardening was assumed isotropic and the hardening behaviour in the building direction was applied to all the different directions. This way, the initial yield surface is anisotropic, but the yield surface expands with the same rate in the different directions. This should not affect results much in Ti-6Al-4V since hardening is low. Nonetheless, it would be straightforward to obtain anisotropic hardening parameters if needed from the stress-strain curves in different directions yielded by the CP model.

Abaqus was used for the macro-scale FEA simulations in this work. Hardening is included in Abaqus plasticity models by specifying the stress values (σ) at different plastic strains (ϵ_p) as tabular data, where ϵ_p is calculated as $\epsilon_p = \epsilon - \epsilon_e = \epsilon_T - \sigma/E$. Here, ϵ_e is the elastic strain, ϵ_T is the true strain and E is the young's modulus, which will correspond to E_{BD} since the flow curve in the BD is used to represent the hardening. To calculate σ and ϵ_p along the flow curve, the stress values at different strains have been calculated by linearly interpolating the flow curve at evenly spaced strain values after the calculated yield strain. This is shown in Figure 57.a), which displays the different hardening points calculated spaced evenly in the strain axis with 0.05% strain increments. Then, an intermediate plastic strain value at each point is calculated as $\epsilon_{pi} = \epsilon - \sigma/E$, but since Abaqus expects a zero plastic strain value for the first input, the first intermediate strain

value is subtracted from all the intermediate strain values ($\epsilon_p = \epsilon_{pi} - \epsilon_{pi_1}$), yielding the final values for ϵ_p . The procedure to obtain the tabular data needed to model hardening in Abaqus is represented in Figure 57.b). The hardening was calculated with this method up to 3.5% post-yield strain; afterwards, it was assumed to be linear with the same rate of change as the last 5 hardening points.

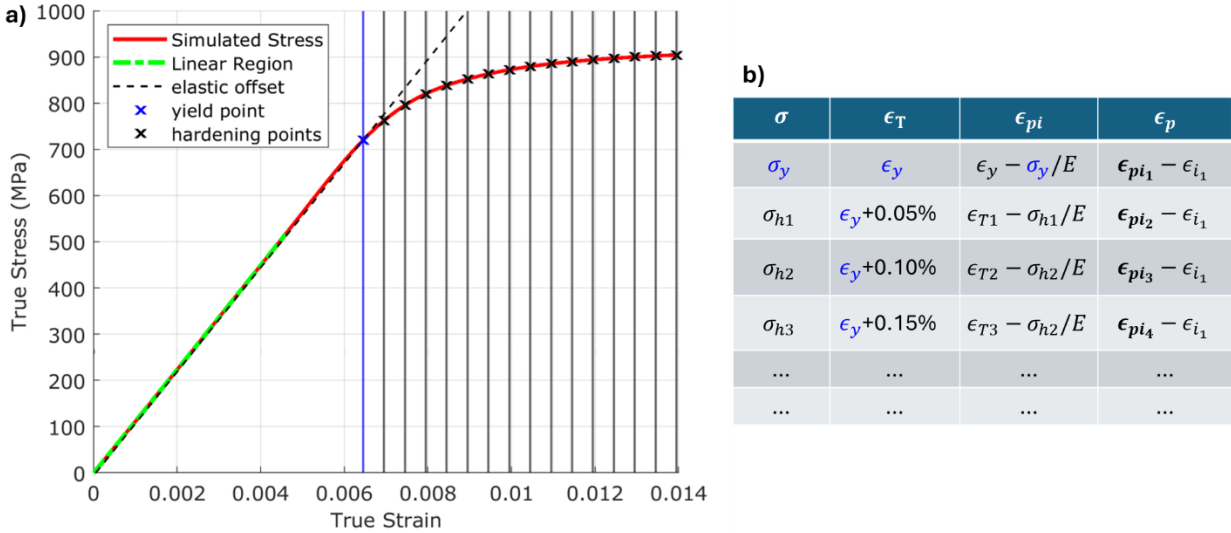


Figure 57. **a)** Calculation of effective elasto-plastic properties from simulated stress-strain curves. It shows how the yield point is calculated using a 0.0005% strain offset of the linear elastic region. It also shows how the hardening is quantified by calculating the stresses at evenly spaced strains after the yield point. **b)** Plasticity parameters in the format required by Abaqus. They are required as tabular data which include stress values σ at different plastic strains ϵ_p . The first point is the yield point, shown in blue as in the graph in **a)**, the rest of the points obtained are the hardening points used to calculate the stresses σ and plastic strains ϵ_p needed.

The orthotropic elastic properties are more straightforward to calculate. The Young Modulus E_X and E_{BD} correspond to the slope of the linearly fitted elastic region in the uniaxial tensile tests, and the shear modulus G_{XY} and G_{BD} are the counterparts in the shear tests. The Poisson's ratios (ν_{XBD}, ν_{XY}) were obtained with the usual formulas using the strains in different directions during the elastic regions of the uniaxial tensile tests ($\nu_{12} = -\epsilon_2/\epsilon_1$).

To sum up, the orthotropic elastic constants and the Hill plasticity parameters for a given set of microstructural parameters ($f_{\alpha'}$, f_{β} , f_{α} , t_{α}) have been calculated by simulating 2 tensile tests and 2 simple shear tests on a digital RVE using the CP model.

5.1.5 Reduced Order Modelling by regression fitting a Structure-Property Database

Due to the high computational expense of CP models, it is not feasible to simulate 4 tensile tests to calculate the local mechanical properties of every material point in the FEA analysis of an AM component. Instead, the interpolation of a structure-property database is suggested in this work, where the data of the structure-property database is generated using the developed CP model. Since the interpolation of a database is much faster than the calculations needed to solve for all the degrees of freedom in numerical simulations, the accelerated model is sometimes referred to as a Reduced Order Model (ROM) or Surrogate Model [203]. These consist of data-driven models trained on the data generated by more computationally expensive models which allow to obtain almost the same results much faster.

The structure-property database for the ROM has been generated through an in-house developed Matlab script, which used the CP model to automatically calculate the desired elasto-plastic properties for different combinations of phase fractions and lath thicknesses. In total, the mechanical properties for 96 different combinations of microstructural parameters were calculated. The combinations included variations for f_{α} and $f_{\alpha'}$ from 0 to 1, for f_{β} from 0 to 0.2 and for t_{lath} from $0.2\mu m$ to $2.7\mu m$. Since each microstructure required 4 tensile test to calculate its properties, as explained in Section 5.1.4, this led to a total of 384 CP simulations. However, since the CP simulations for different microstructures can be run independently from each other, the code could run in parallel, which decreased the time required to generate the database significantly. Parallel for loops using *parfor* in Matlab allowed to easily perform this task [204]. By parallelising the RVE generation, CPFFT simulations and property calculations, the computations of the database generation lasted around 3 days using 24 cores, which is a reasonably short time considering that it only needs to be done once. Therefore, it is feasible to extend this database in the future for more complex yield curves or more microstructural combinations. A link to the repository of the code used to generate the database can be found in Appendix A.4.

Thereafter, regression models were developed for each effective property calculated (σ_{xx}^y , σ_{BD}^y , E_X , ν_{XY} ...), as well as for each hardening point. For the hardening points, only the stress values were fitted. For the strain values, with the methodology used to calculate the hardening points from the flow curve (see Section 5.1.4.), they can be quantified as the strain difference to the yields point ($\epsilon^* = \epsilon_T - \epsilon_y$), which would be the same for all microstructures.

The fitting was carried out using a multi-variate polynomial regression of 3rd degree using the scikit-learn Python library [205]. In order to test the interpolation method, a validation dataset was generated using the same procedure as for the database but for microstructural values which were not already in the database. Then, the normalised differences in property values between the validation dataset and the fitted quantities were calculated and used as an estimate of the error in the regression. Interpolation methods such as linear interpolation or Radial Basis Function (RBF) interpolation as well as different polynomial degrees were also tested with this approach. The computed average errors for some of the methods analysed are displayed in Table 9. Linear and RBF interpolation yielded slightly lower errors than polynomial regression but are more computationally expensive to evaluate. Higher polynomial degrees than 3 produced slightly lower errors, but were not adequate for the 96 datapoints used, leading to very large fitting coefficients which could lead to floating point errors. For these reasons, a polynomial with degree 3 was used.

Table 9. Average errors of the different machine learning approaches tested to produce a ROM of crystal plasticity simulations for the structure-property model.

ROM Method	Avg. Error (%)	Max. Error (%)
Linear regression	1.4	3.13
Polynomial regression degree 2	1.5	2.7
Polynomial regression degree 3	0.98	1.79
Polynomial regression degree 4	0.30	0.65
Linear Interpolation	0.20	0.55
RBF Interpolation	0.11	0.32

Polynomial regression consists of fitting an analytical function f for every property p as a function of the microstructural parameters $f_\alpha, f_{\alpha'}, f_\beta, t_{lath}$ through a set of fitting parameters

$\mathbf{x} = x_0, x_1, \dots, x_n$. This is represented in Equation 35 for a polynomial of degree 2. $f_{\alpha'}$ is not included because it can be calculated from f_{α} and f_{β} through $f_{\alpha'} = 1 - (f_{\alpha} + f_{\beta})$, which is linearly related without affecting the results. The fitting parameters $\mathbf{x}$ are calculated through an ordinary least-squares optimisation process using scikit-learn. The higher the degree of the polynomial fit, the higher the number of parameters and the obtained function will be more non-linear. However, high degrees can lead to overfitting and large coefficients, producing larger regression errors. A polynomial of degree 3 was chosen for the polynomial regression of the different properties computed.

$$p(f_{\alpha}, f_{\beta}, t_{lath}) = x_0 + x_1 * f_{\alpha} + x_2 * f_{\alpha}^2 + x_3 * f_{\beta} + x_4 * f_{\beta}^2 + x_5 * t_{lath} + x_6 * t_{lath}^2 + x_7 * f_{\beta} * f_{\alpha} + x_8 * f_{\alpha} * t_{lath} + x_9 * f_{\beta} * t_{lath} \quad \text{Equation 35}$$

With the proposed ROM consisting of the regression fitting of a structure-property database generated with CP simulations, the properties for many different microstructures can be rapidly computed. This allows to quickly calculate the local mechanical behaviour along an AM component if its microstructure is known throughout it. A link to code of the developed structure-property ROM can be found in Appendix A.5.

5.2 Experimental Methods

5.2.1 Tensile testing

To analyse the predictive capabilities of the developed structure-property model, the results were compared and contrasted with experimental tensile tests of additively manufactured Ti-6Al-4V samples with different microstructures.

Miniaturised tensile test specimens were extracted at different layer heights of cuboids manufactured in-house with different process parameters. The manufactured cuboids were those discussed in detail in Chapter 4, where more information on the manufacturing methodology can be found. Three tensile specimens were extracted from each cuboid by means of EDM. The specimen geometry as well as the schematic positioning of the specimens inside a cuboid are shown in Figure 58. The phase fractions and lath thicknesses of each specimen were measured in

Chapter 4 using SEM in BSE mode followed by quantitative image analysis using MIPAR software.

Table 10. Summary of the process parameters used for in-house manufacturing of each cuboid.

Manufacturing Process Parameters Applied for each Cuboid	
C1-B1	Baseline process parameters
C2-B2	Half-hatch spacing and rescanned each layer one time with full power
C3-B2	Rescanned each layer one time with full power
C4-B3	Rescanned each layer 6 times with $\frac{3}{4}$ of the baseline power
C5-B3	Rescanned each layer 6 times with $\frac{1}{2}$ of the baseline power
C3-B2-HT800	C3 + heat treated at 800 °C for 2 hours followed by furnace cooling
C5-B3-HT850	C5 + heat treated at 850 °C for 2 hours followed by furnace cooling

The uniaxial tensile tests were performed at room temperature under a nominal strain rate of $\dot{\epsilon} = 2 \cdot 10^{-4} \text{ s}^{-1}$. An electro-thermal mechanical testing (ETMT) system developed by Instron (Instron™ ETMT 8800©) was used because it allowed for miniaturized specimens to be tested. The strain was measured using Digital Image Correlation (DIC) using a 3D DIC system (LaVision's MX4M digital cameras installed on a Zeiss Discovery V12 3D stereo microscope). A fine speckle pattern was produced on the surface in the area of interest using a white high-temperature paint as a background with an overspray of a black paint of the same type. The area of interest was $2 \times 2 \text{ mm}$, with a frequency of imaging of 1 Hz . The rest of the tensile testing procedure is identical to what is reported in ref. [206], which provides a detailed description of the technique and its accuracy.

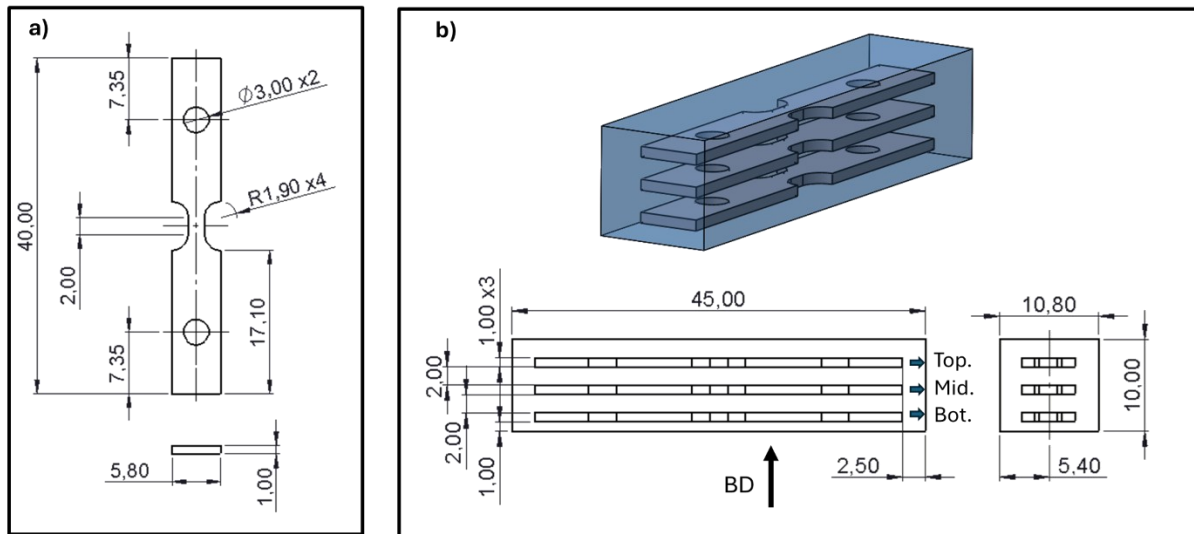


Figure 58. **a)** CAD model showing the geometry of the dogbone specimens used for the in-house tensile tests to validate the structure-property model. **b)** CAD showing the positioning of the tensile test specimens inside the additively manufactured cuboids.

5.2.2 SEM and EBSD

For the explanations of the AM microstructures that are to be investigated in this work and the assumptions taken to model them, microstructure characterisations were carried out to obtain quantitative microstructural information for the models, as shown in Figure 52 and Figure 55 and explained in Section 5.1.2. To obtain this information, some of the cuboids were machined using wire EDM and prepared by conventional metallographic methods to mirror finish conditions.

Characterisations were performed using SEM in backscattered electron (BSE) mode and electron back-scattered diffraction (EBSD). An accelerating voltage of 10 *kV* was used for the BSE images and 15 *kV* for the EBSD map. The system used consisted of an FEI Quanta-250 SEM interfaced with a fully automated Aztec HKL Advanced (plus C5 Prem) Nordlys Max 2 EBSD system. The EBSD measurements covered an area of $\approx 3.0 \times 3.1\text{mm}$ with a step size of $2.5\text{ }\mu\text{m}$. The EBSD map was measured on sample C5-B3-HT850, since the heat treatment allowed for easier indexing, i.e., leading to $\approx 82\%$ of indexed points. This is because it produces larger lamellae with less distorted lattices without modifying the PBG structure, which was the main interest of the analysis.

5.3 Results and Discussion

5.3.1 Analysis of Structure-Property Relations from Experimental Tensile Tests

This subsection contains a purely theoretical analysis of the structure-property relations that can be inferred from the experimental tensile tests and microstructural analysis performed in this work. Figure 59 shows the tensile test results for the different samples tested in this work. Table 11 displays the measured microstructural features in the different samples. As can be seen in Figure 59, the samples extracted from the same cuboid (i.e., shown by the same colour in the plot) have displayed very similar flow behaviours, with the exception of sample C3-B2-HT800-B. Looking at the measured microstructural features in Table 11 for each sample, it can be seen that all the samples that belonged to the same cuboid have very similar characteristics. Therefore, it is unlikely that the outlying behaviour from sample C3-B2-HT800-B is explained by its microstructure, being most likely caused by a difference in porosity or damage during the machining to extract it from the cuboid. For this reason, the results from C3-B2-HT800-B will be ignored for the rest of the microstructure-focused discussion.

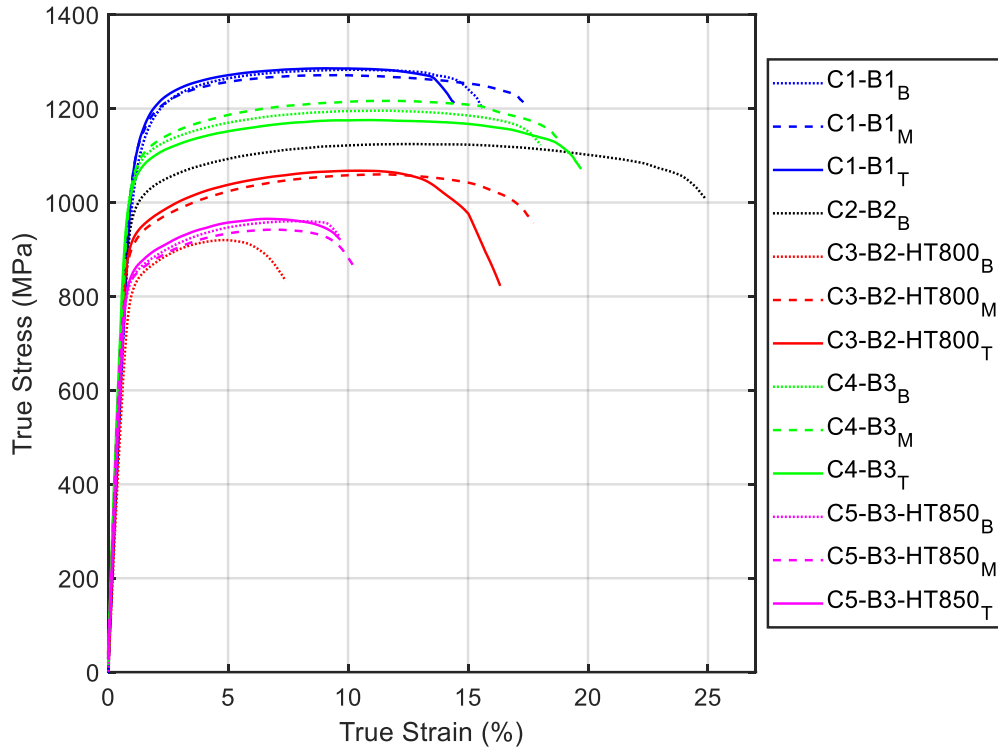


Figure 59. True tensile stress-strain curves for the LPBF Ti-6Al-4V samples extracted from the cuboids manufactured with different process parameters in this work. The samples that belong to the same cuboid have been plotted with the same colours. The process parameters used to manufacture each cuboid are explained in Table 6 of Chapter 4. The microstructural parameters measured for each cuboid are provided in Table 11.

Table 11. Microstructural parameters measured in the tensile test samples in Chapter 4. For the heat-treated samples in the cuboids C3-HT800 and C5-HT850 only an average measure of the 3 samples is provided since the microstructure was homogeneous along the entire cuboid.

Sample Name	f_{β} (%)	f_{α} (%)	$f_{\alpha'}$ (%)	t_{α} (μm)
C1-B1-Bot	0	0	100	-
C1-B1-Mid	0	0	100	-
C1-B1-Top	0	0	100	-
C4-B3-Bot	2.5 $\pm$ 2.1	48 $\pm$ 2.1	50	0.30 $\pm$ 0.05
C4-B3-Mid	4.3 $\pm$ 3.1	45 $\pm$ 3.1	50	0.30 $\pm$ 0.03
C4-B3-Top	4.0 $\pm$ 2.0	46 $\pm$ 2.0	50	0.29 $\pm$ 0.05
C2-B2-Bot	8.1 $\pm$ 2.3	92 $\pm$ 2.3	0	0.33 $\pm$ 0.03
C3-B2-HT800	6.0 $\pm$ 1.3	94 $\pm$ 1.3	0	1.0 $\pm$ 0.1
C5-B3-HT850	7.2 $\pm$ 0.6	93 $\pm$ 0.6	0	1.3 $\pm$ 0.1

The samples behaved as expected from their microstructure according to the literature. A higher amount of martensite increased strength, as seen for the samples in C1-B1 ($f_{\alpha'} \approx 100\%$), manufactured with the baseline process parameters which yielded a fully martensitic microstructure. The higher the intensity of heat supplied during the build the higher the martensite decomposition and therefore the lower the strength. This can be seen for C4-B3 ($f_{\alpha'} \approx 50\%$) and C2-B2 ($f_{\alpha'} \approx 0\%$) which have lower strengths. C4-B3 was partially decomposed while C2-B2 showed a full decomposition, therefore the former was stronger than the latter, but both had less strength than C1-B1 ($f_{\alpha'} \approx 100\%$) with a fully martensitic microstructure. For fully decomposed samples (C2, C3-HT800, C5-HT850), larger lath thicknesses (t_{α}) led to lower strength, as expected from the Hall-Petch effect. The heat-treated samples had much higher t_{α} and showed significantly lower strengths. Overall, for strength, the more heat delivered to the material by means of changing the process parameters or the heat treatments, the lower the strength became.

However, the relationship between heat input and ductility was not as straightforward, as increasing heat did not simply increase ductility. For the as-built samples, more heat decomposed the martensite into thin lamellar $\alpha + \beta$, which resulted in increased ductility. However, for the heat-treated samples, where significantly more heat was supplied to the material leading to coarsen microstructure, the ductility decreased, which was measured to be lower for a higher heat treatment temperature. The low ductility in heat-treated samples could be attributed to the formation of Grain Boundary α (GB- α). GB- α refers to elongated α grains that form along the PBGs during slow cooling near β transus temperature. The presence of GB- α has been captured in the heat-treated samples by SEM (i.e., BSE imaging mode), as highlighted in Figure 60. GB- α , especially the continuous GB- α present in these samples, is reported in the literature to significantly decrease ductility [207, 208]. This is because they are softer grains that produce strain concentrations while also allowing for easier crack propagation, i.e., no obstacle to crack growth over a long path with no GBs or β lamellae. Both effects are not captured by the phenomenological CP model used. These effects are even more pronounced in these tests as the samples are loaded perpendicular to the BD, and since the PBGs are columnar and aligned towards the BD, the GB- α is perpendicular to the loading direction and therefore the cracks will have a tendency to propagate faster.

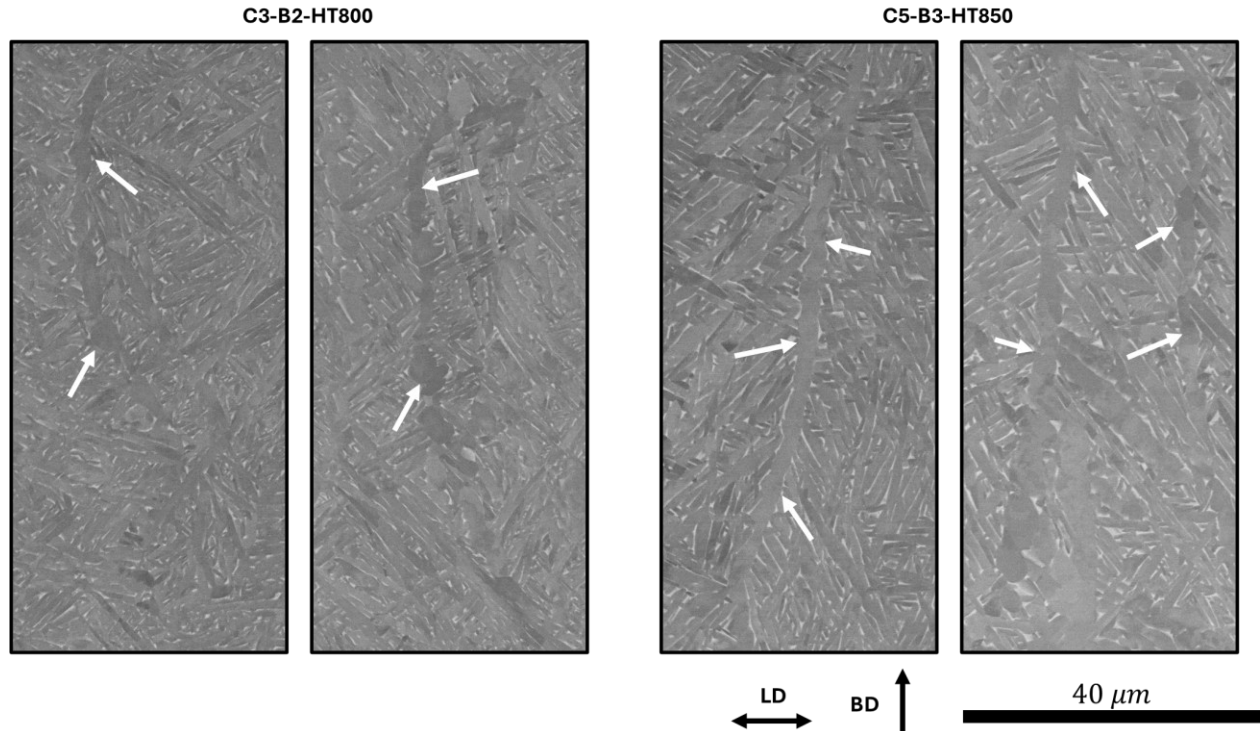


Figure 60. SEM BSE images of the heat-treated samples showing the appearances of GB- α . Two examples are shown for each cuboid. The white arrows point towards the GB- α grains. The dark arrows show the Building Direction (BD) and the Loading Direction (LD).

Therefore, there seems to be an optimal degree of heat that can be supplied to the material in order to produce the best ductility. This amount of heat could likely be controlled through model-based optimisation of the process parameters using the process-structure model from Chapters 3 and 4. This would allow to guarantee a homogenous optimal microstructure, which the author would like to suggest as future work.

This also shows that the developed structure-property model in this work, which is limited to predict strength and not ductility, cannot really be used to calculate the optimal microstructure. Therefore, it would be useful in the future to extend the current structure-property model to predict changes in ductility as a function of microstructural parameters. It is likely that this will require to add damage initiation and propagation in the CP model, as well as the addition of GB- α grains to the RVE.

Nonetheless, at the current state of the art where it is not yet straightforward to predict ductility confidently with CP models, predicting strength can still be useful as it is the property usually used in structural design to optimise components with FEA.

5.3.2 Experimental Validation of the CP Model for Stress-Strain Predictions

Figure 61 compares the predicted tensile flow curves using the CP model with experimental curves from different cuboids. To simplify the analysis, since all the samples from the same cuboid had similar flow curves and microstructures, the experimental flow curves for a given cuboid have been averaged, only yielding one flow curve per cuboid. Then, the simulated flow curves for each cuboid were obtained using averaged microstructure parameters as input to the CP model.

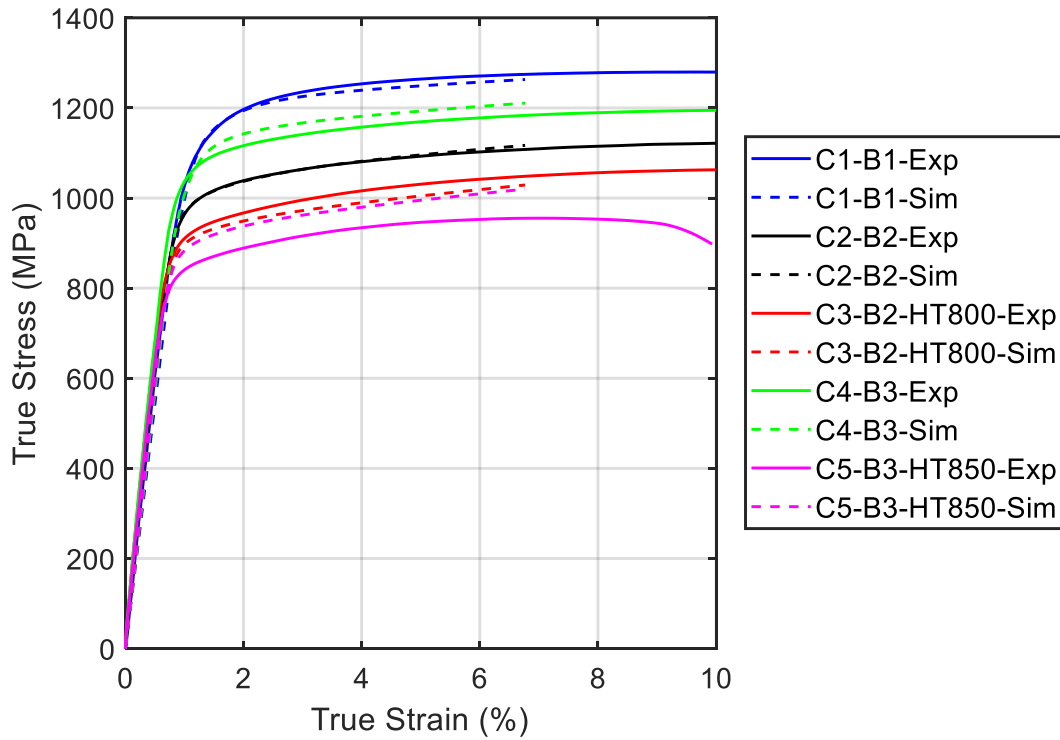


Figure 61. Comparison between experimental tensile stress-strain curves and simulated curves from CP simulations for cuboids manufactured with different process parameters. The experimental curves represent averages of different tensile tests on samples extracted from each cuboid. The simulated curves were obtained using averaged microstructural parameters as inputs to the CP model.

Figure 61 shows a good match for all cuboids except for sample C5-B3-HT850. It seems that this sample did not follow the Hall-Petch relationship that was apparently followed by the other $\alpha + \beta$ samples. This effect could be attributed to the long and continuous GB- α present in this cuboid, displayed in Figure 60, as it has been shown to decrease strength [209]. Some other significant

sources of error could be porosity and residual stress. Porosity was verified to be below 0.1% by optical methods, but maybe some pores inside the samples were missed and nano-scale pores cannot be seen by optical methods. Residual stress should mostly be removed during machining of the tensile specimens, but it is likely that some residual stress remained in the tensile specimens. Furthermore, residual stress could produce distortions during machining that can lead to different surface finishes on the tensile test specimens. Both porosity and residual stress could also be affected by changes in process parameters undertaken for different cuboids. Finally, another source of error could be changes in composition with different process parameters through the evaporation of Al. Though, this is not usually a problem in AM of Ti-6Al-4V as opposed to other alloys [40].

Overall, nonetheless, the model yielded acceptable accuracy for predicting as-built material properties, where GB- α is not expected. It must be noted as well that the CP parameters were calibrated using samples loaded parallel to the BD direction, while the validation samples were loaded perpendicular to the BD, showing that anisotropy is captured as well. An analysis of the anisotropy prediction is shown in Section 5.3.4.

Coupling the current model with chemical, porosity and residual stress prediction models would be a good future development to increase the fidelity of the PSP model. Nonetheless, the author estimates that the largest error is due to the GB- α , which is formed during very slow post heat treatment cooling rates and is not usually seen in as-built LPBF samples, for which this model is meant. Therefore, the current model should still be quite accurate for as-built LPBF samples or for heat-treatments that avoid significant GB- α .

5.3.3 Effective Macro-scale Properties Prediction

The overall objective of this thesis is to include the effect of microstructural heterogeneity in the structural FEA modelling of AM components. This has been accomplished by extracting effective properties from simulated tensile tests of RVEs of different microstructures using CP, as explained in the methodology. This section showcases the accuracy of the calculated macro-scale effective properties predicted by using the flow curves obtained via the CP model, as well as the accuracy of the ROM which calculates these properties “instantly” through fitting a structure-property database. For this, the stress-strain behaviour obtained from macro-scale FEA simulations in Abaqus with the calculated properties has been contrasted with the initial flow curves from the CP simulations.

The validation of this approach (i.e., property calculation) is performed through an elasto-plastic model in Abaqus, which includes all of the effective material properties calculated with the methodology described in **Section 5.1.4. Calculation of Effective Macro-Scale Properties**; these are orthotropic elastic properties, Hill plasticity and isotropic hardening. Thereafter, this material model is applied to uniaxial loading simulations using a single element. A 3D hexahedral linear element with reduced integration was used (C3D8R). If the stress-strain curves taken from the CP simulation of the RVE and the results of the Abaqus simulations match, it implies that the effective properties extracted from the CP results are correct and that they can be used in the FEA modelling of macro-scale components.

Figure 62 shows two sets of flow curves, each for a different microstructure loaded in the BD with a given set of phase fractions and α lath thickness (i.e., values are provided in the Figure's caption). For each set, there are three flow curves, one corresponding to the curve predicted by the CP model (red), one corresponding to the single element simulated in Abaqus using the properties directly extracted from the CP results (blue), and a flow curve also from the Abaqus simulation using the properties predicted by the ROM through database interpolation (yellow). It can be seen that for both microstructures, the three flow curves display very similar results.

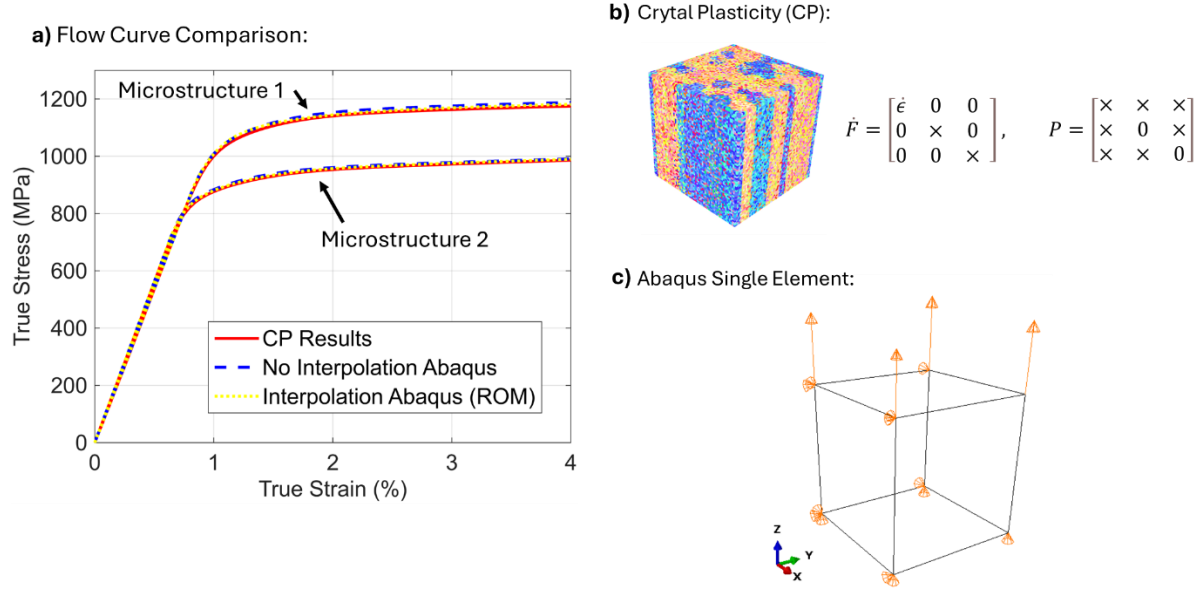


Figure 62. Validation of the predicted effective properties through Computational Homogenisation. **a)** Two different sets of three flow curves corresponding to two different microstructures tested in the BD. Microstructure 1 had microstructural values of $t_\alpha = 0.4$, $f_\alpha = 0.33$, $f_\beta = 0.09$ and Microstructure 2 had values of $t_\alpha = 1.42$, $f_\alpha = 0.88$, $f_\beta = 0.12$. These values were chosen arbitrarily. For each set of flow curves, one corresponds to the data extracted from the CP model (red), one extracted from the single element test simulated in Abaqus using the properties directly extracted from the CP flow curve (blue), and one from the single element with properties obtained with the ROM by interpolation of a structure-property database (yellow). **b)** Example RVE and BCs used in the CPFFT model of uniaxial tensile test. **c)** Single Element and BCs used in the FEA Abaqus simulations.

The flow curves predicted via the single element simulation, i.e., without interpolation (blue), show slightly higher stresses, which is expected due to the linear offset applied when calculating yield stress. However, the difference is very much negligible, showing that the flow curves obtained by CP simulation are good enough to be used in Abaqus for the macro-scale FEA simulations. For the flow curves predicted in Abaqus by using the ROM, which interpolates the structure-property database, the differences with the CP results are also very small. This means that the automatic generation of a structure-property database is working effectively, and that the ROM regression method of multivariate polynomial regression provides an accurate estimate of the elasto-plastic properties for a given set of microstructural parameters (i.e., $f_\alpha, f_\beta, f'_\alpha, l_{th}$).

5.3.4 Structure-Property Database Analysis

Although the aim of this thesis is to study the feasibility of a PSPP model for manufacturers to optimise structural AM components, analysing the generated structure-property database also allows to derive some scientific conclusions on the effect of Ti-6Al-4V microstructure on elasto-plastic properties. Furthermore, by comparing the obtained conclusions with equivalent experimental conclusions in the literature, the fidelity of the developed modelling approach can be analysed. Figure 63 shows the effect of microstructural parameters on the yield strength for different loading directions. In the scatter plots of Figure 63.a), each point corresponds to a different microstructure in the structure-property database.

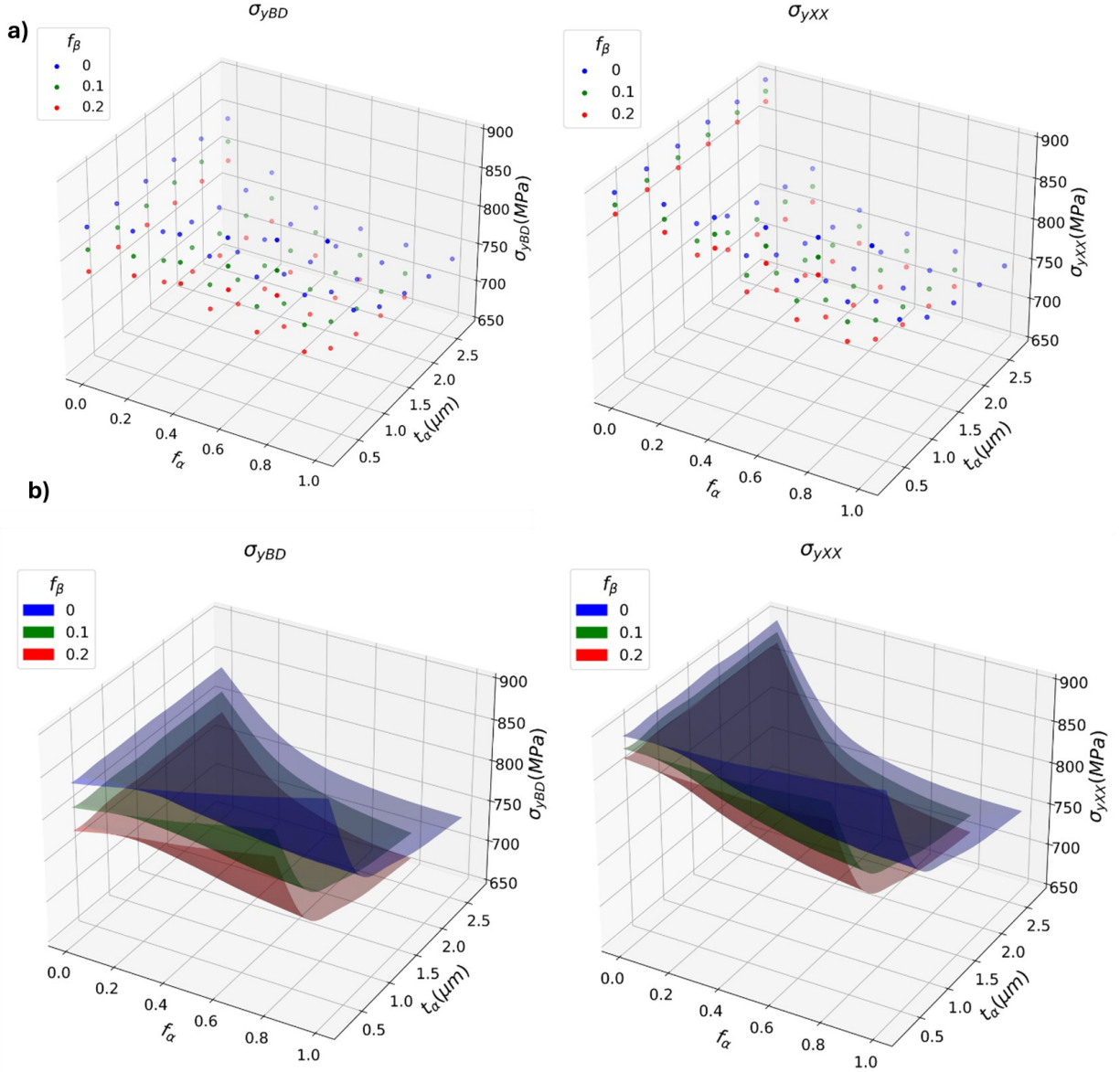


Figure 63. Effect of microstructure on yield strength of AM Ti-6Al-4V in different loading directions predicted by the CP model. **a)** Scatter plots of yield strength as a function of microstructure parameters containing all the microstructures simulated to generate the structure-property database. The left plot corresponds to yield stress in the BD (σ_{yBD}) and the right plot to yield stress in the horizontal direction (σ_{yXX}). The colours correspond to different f_β values as shown in the legends, $f_{\alpha'}$ corresponds to $f_{\alpha'} = 1 - f_\alpha - f_\beta$, so its magnitude can be understood from the other phase fractions and has not been included in the plots. **b)** Surface plots consisting of a spline interpolation of the same data in **a)**, showing a surface for each value of f_β . These plots allow for better visualisation of the effect of microstructure on yield strength.

From the scatter plots, three different surfaces were generated as displayed in Figure 63.b), where each surface has a constant value of f_β and allows to better understand microstructural effects on yield strength. Looking at the surface plots, the following conclusions can be drawn:

- A higher amount of β phase decreases yield strength; this can be seen as the surfaces corresponding to lower f_β fractions are higher in Figure 63. This effect is widely known in Ti alloys, as the BCC β crystals better accommodate plasticity and start to yield at lower stresses compared to the HCP α/α' phases [210].
- Smaller α lath thickness (t_α) increases yield strength following an asymptotic behaviour. This is expected from the Hall-Petch effect, and the square root expression used to modify the critical resolved shear stress τ_0 as a function of lath thickness shown in Equation 27. This effect was seen in the tensile tests from Figure 59 and has been reported experimentally for Ti-6Al-4V in several studies [141, 150, 211]. Future CP models should intend to predict this physically by modelling dislocation transmission, which would allow digital microstructure optimization and more accurate simulations.
- When martensite increases (f_α and f_β decrease) the yield strength increases, but this effect is much lower when the α lath thickness t_α is low. This has also been seen in the tensile tests shown in Figure 59 and reported by Xu et. al. in ref. [211], where they produced a very thin lamellar $\alpha + \beta$ microstructure by decomposing martensite, which yielded lath thicknesses similar to the martensitic microstructure. When experimental tensile tests were performed, both the martensitic and thin $\alpha + \beta$ microstructure yielded similar strengths due to the small grain size of the $\alpha + \beta$ microstructure.

The effects of microstructure effects on yield strength predicted by the CP model can all be corroborated with the literature, which gives confidence in the predictions of the developed CP model. This also shows that a similar CP model and database generation procedure could be used to analyse phase and grain size effects on strength for novel alloys, where there is no previous experimental analyses, and the outcomes save resources on experimental costs.

Regarding anisotropy, one of the main benefits of computational homogenisation with CP models is that it accounts for the effect of texture on yield strength anisotropy. This is because CP considers the crystallographic anisotropy of each grain and therefore the effect of the Schmid factor and CRSS of each slip system in the global response of the RVE. As the effect of microstructural texture on mechanical anisotropy was not shown clearly in Figure 63, similar surface plots using

the ratio of stresses $\sigma_{yXX}/\sigma_{yBD}$ were generated instead, which is displayed in Figure 64. The plot show that for all the microstructures, the yield strength is around 2 to 10% higher when the load is horizontal (perpendicular to the BD), which is common for Ti-6Al-4V made by AM, and has been measured experimentally and reported in several references [212-214].

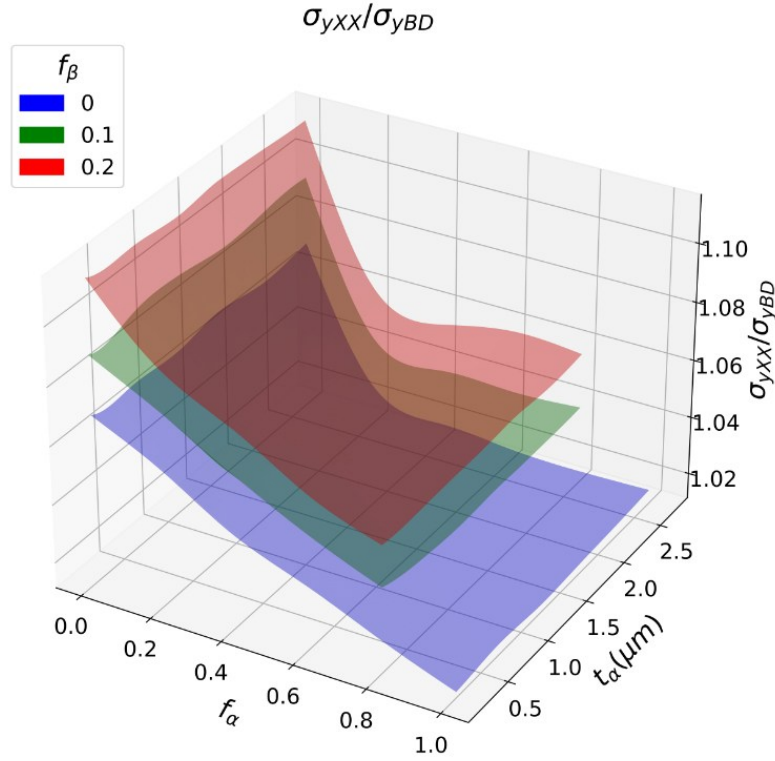


Figure 64. Ratio of yield stresses in perpendicular loading directions ($\sigma_{yXX}/\sigma_{yBD}$) as a function of microstructural parameters to display effect of microstructure on tensile strength anisotropy.

Regarding the effect of microstructure, when f_β increases, the anisotropy increases, which is clearly seen in the figure as the red surface ($f_\beta = 0.2$) is at the top. This can be attributed to the higher texture of PBGs in contrast to α/α' grains. When the material solidifies with a high gradient during AM, it forms very large and textured columnar β grains. However, when it cools down, the β grains transforms to α/α' , i.e., each β grain has a chance to transform to 12 different variants (see IPFs in Figure 52). This weaker texture is likely to decrease tensile anisotropy when there is less quantity of β .

The anisotropy has a more complex relationship with $f_{\alpha'}$, which is attributed to the differences in critical resolved shear stresses (τ_0) along the slip systems of α and α' . This should

also explain the low effect of t_α , since the ratios between slip systems are independent of t_α . A deeper analysis of these effects could be performed in future by analysing the Schmid factors for each slip system and their τ_0 . As the overall variation of yield stress anisotropy with microstructure in AM Ti-6Al-4V is fairly low, there are not studies published on this matter in the literature and could not be verified experimentally at the moment.

Overall, the CP model yields reasonable estimates of anisotropy. Nonetheless, with further comparison with experimental results, the current structure-property model shows some limitations. Yang et. al. produced a detailed study of the tensile anisotropy in PBF of Ti-6Al-4V for samples printed with different energy densities [215], whose results are shown in Figure 65. In these plots, they reported a higher ultimate and yield strength when loading the samples perpendicular to the BD, as predicted by the CP model. However, they showed that yield strength difference ratio (YDR) increases with energy density, meaning that it changed the anisotropy in yield strength. They attributed these differences in strength anisotropy to changes in the texture of α/α' when the energy increases, which better favours slip in the weak prismatic systems. This effect should be captured by CP models, but it is not captured in the current process-structure-property model as a constant $\langle 100 \rangle$ fibre texture is assumed in the PBGs. Furthermore, they reported notable differences in the elongation to failure between the loading directions, which are attributed to damage initiation and propagation and cannot be captured either in the current CP model. These are two possible areas for improvement in the future for the process-structure-property models of AM.

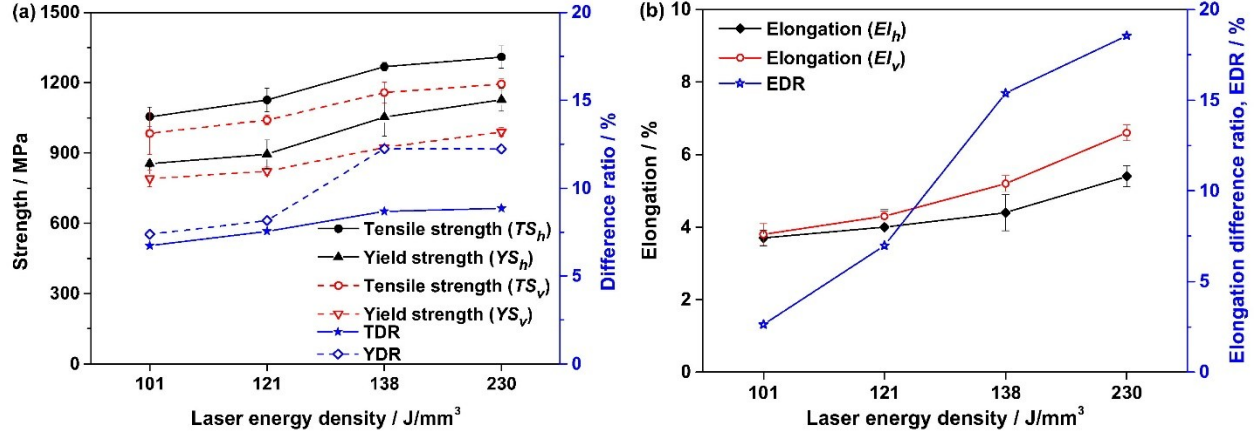


Figure 65. Tensile properties of PBF Ti-6Al-4V as a function of energy density in the vertical (BD) and horizontal directions. **a)** Ultimate tensile strength (TS) and yield strength (YS) in the horizontal (h) and vertical (v) directions and the anisotropic difference ratios for different energy densities. TDR is the TS Difference Ratio and YDR is the YS Difference Ratio, which are measures of anisotropy. **b)** Elongation to failure in the vertical and horizontal directions, as well as the Elongation Difference Ratios (EDR), for different energy densities. Figure reproduced from ref. [215].

5.4 Summary and Conclusions

A structure-property model for Ti-6Al-4V built by AM has been developed that predicts tensile flow curves in different directions as a function of several microstructural characteristics. These parameters are namely the phase fractions of α (f_α), β (f_β) and α' ($f_{\alpha'}$); as well as the lath thickness of α (t_α). These parameters can be predicted by the microstructure evolution model developed in **Chapter 4** and are the ones that mostly influence the strength of AM Ti-6Al-4V.

The model consists of a computational homogenisation approach by performing CP simulations of tensile tests in different directions on a microscopic RVE. For a given RVE that represent a microstructure with specific parameters ($f_\alpha, f_\beta, f_{\alpha'}, t_\alpha$), arbitrary tensile tests can be performed with this approach to obtain its anisotropic tensile properties ($E_{XX}, E_{BD}, \sigma_{yXX}, \sigma_{yBD}$).

However, if this model is to be used to calculate the properties throughout a component with very heterogeneous microstructures, it is not feasible to run expensive CP models for every point to know its properties. To solve for this, a Reduced Order Model has been developed by fitting a database which relates local microstructural characteristics ($f_\alpha, f_\beta, f_{\alpha'}, t_\alpha$) to mechanical response ($E_{XX}, E_{BD}, \sigma_{yXX}, \sigma_{yBD}$) with a data-driven regression model. This regression model then allows to calculate the properties of a given microstructure instantly and quickly know the local

mechanical properties along a component if its local microstructural properties are known. This is especially useful to populate local mechanical properties throughout a component using FEA for structural performance analyses. The developed regression model showed a very low level of uncertainty against a validation dataset, meaning that it can reproduce the results of the expensive CP model with high fidelity. The obtained predictions were also imported into Abaqus and were shown to reproduce the same tensile behaviours as those of the CP model.

When analysing the predictive capability of the developed models against experimental results, the following conclusions can be made:

- Overall, the CP model predictions correctly matched the experimental tensile tests for different microstructures. However, some important deviations were seen. These were mostly attributed to the appearance of GB- α ; but porosity, local chemical heterogeneities and residual stress might have also affected the results. These effects are not currently captured in the CP model. Including these phenomena in the model in the future could be beneficial.
- The CP model correctly estimated the yield strength anisotropy of AM Ti-6Al-4V, which predicted around 5% lower strength in the BD, similar to what is reported in the literature. The model also predicted variations between 2% to 10% in yield strength anisotropy depending on the microstructure. However, the effect of microstructural parameters on yield strength anisotropy could not be verified experimentally as the deviation is low, making it hard to measure, and therefore no experimental studies were found on this matter.
- The CP correctly captured the effect of phase fractions and lath thickness on yield strength. Furthermore, the model predicted that when the lath thickness of α is low enough, its strength is similar to a fully martensitic (α') microstructure, which has also been reported in the literature.
- The literature shows a very high anisotropy in ductility attributed to the columnar β grains and GB- α . This cannot be captured by the CP model in this work, as it depends on damage initiation and propagation. Adding these physics in the future to the CP model could be very useful for PSPP models of AM. If ductility is to be included in PSPP model, it is likely that the prediction of GB- α will need to be included in the microstructure evolution model.
- The literature shows that AM scanning parameters can affect texture and therefore anisotropy. The current structure-property model assumes a constant texture as it cannot

be captured by the previously developed microstructure evolution model. Predicting texture, for example with CA models, and including its effect in the structure-property model should be studied in the future.

- Surface roughness has been ignored in this study, as tensile tests were machined. Surface roughness can be significant in AM and can have an impact on properties. Studies of how to include this in structure-property models could also be beneficial.

6. PROCESS-STRUCTURE-PROPERTY-PERFORMANCE MODELLING OF ADDITIVELY MANUFACTURED TI-6AL-4V

In the previous **Chapters 3 to 5**, different computational models addressing several physics that influenced the mechanical properties of AM Ti-6Al-4V were developed and their accuracy was analysed experimentally. Firstly, a thermal FEA model of the AM process to yield local temperature histories was developed in **Chapter 3**. Secondly, in **Chapter 4**, an analytical mean-field microstructure evolution model was proposed to calculate the phase fractions and lath thicknesses from a given thermal history. Finally, a microstructure-property model was produced in **Chapter 5** that calculated elasto-plastic properties as a function of microstructural features. Although these models were developed in this thesis with the objective of using them for process-structure-property-performance modelling, it made sense to split them in different chapters since they modelled different physics and could be used independently from each other for different purposes.

Ultimately, this chapter presents the development of the Process-Structure-Property-Performance (PSPP) modelling approach. It integrates the previously developed models with structural FEA simulations to account for the effects of the additive manufacturing process on microstructure evolution and the resulting mechanical performance. The proposed approach overcomes limitations of conventional structural FEA models for Ti-6Al-4V, which typically assume constant mechanical properties, ignoring the effect on properties from the process parameters and component geometry. By accounting for these factors, the structural performance of additively manufactured components can be assessed more accurately, while also enabling simultaneous optimisation of both geometrical design and manufacturing parameters.

This chapter begins by outlining the methodology of the proposed modelling approach. Subsequently, an application example is presented in which the compression of a lattice structure is simulated, incorporating the effects of additive manufacturing on local mechanical properties. The results are then compared with experimental data from the literature to analyse the accuracy and limitations of the developed model.

6.1 Methodology of PSPP Model of AM Ti-6Al-4V

A schematic representation of the developed PSPP model is shown in Figure 66. The primary inputs to the model are a CAD geometry of the AM component and the process parameters used for the AM process to manufacture the part. In this manner, all the relevant information pertaining to both the design and manufacturing of the component is accounted for in the estimation of its structural performance.

These inputs are utilised by the thermal process FEA model introduced in **Chapter 3** to compute temperature histories throughout the entire AM process. Specifically, the CAD geometry serves as the basis for defining the computational domain of the thermal model, i.e., via the generation of appropriate meshes. The process parameters encompass all variables required by the PBF system to execute the AM process, which directly influence the thermal history of the material. These include, for instance, the laser power, scan path, and layer thickness. A detailed discussion on the role and impact of the CAD model and process parameters is provided in **Chapter 3**.

The resulting temperature histories at selected spatial locations are subsequently used as input for the microstructure evolution model described in **Chapter 4**. This model is based on a mean-field approach that employs a set of analytical equations to predict the evolution of key microstructural features in Ti-6Al-4V relevant to structural performance. These are namely the lath thicknesses and phase fractions of α , α' and β ($f_{\alpha'}$, f_{β} , f_{α} , t_{α}).

The microstructural parameters derived at each location are then input into the structure-property model presented in **Chapter 5**. This model is a Reduced Order Model (ROM) trained on a series of full-field CP-FFT simulations of tensile tests conducted in multiple directions. The ROM facilitates a rapid estimation of orthotropic elasto-plastic properties from microstructural input. Specifically, the obtained properties are the orthotropic Elastic constants (E_{ij} , ν_{ij} , G_{ij}), orthotropic Hill plasticity yield surface $\sigma_{y_{ij}}$ and isotropic hardening.

Subsequently, the computed local properties are mapped onto a different FEA mesh of the input CAD geometry specific to structural analysis. This FEA mesh with local mechanical properties assigned is finally exported in a format compatible with Abaqus such that it can be imported to develop arbitrary structural FEA simulation of the component to analyse. The software framework developed to perform these operations automatically can be accessed in Appendix A.6.

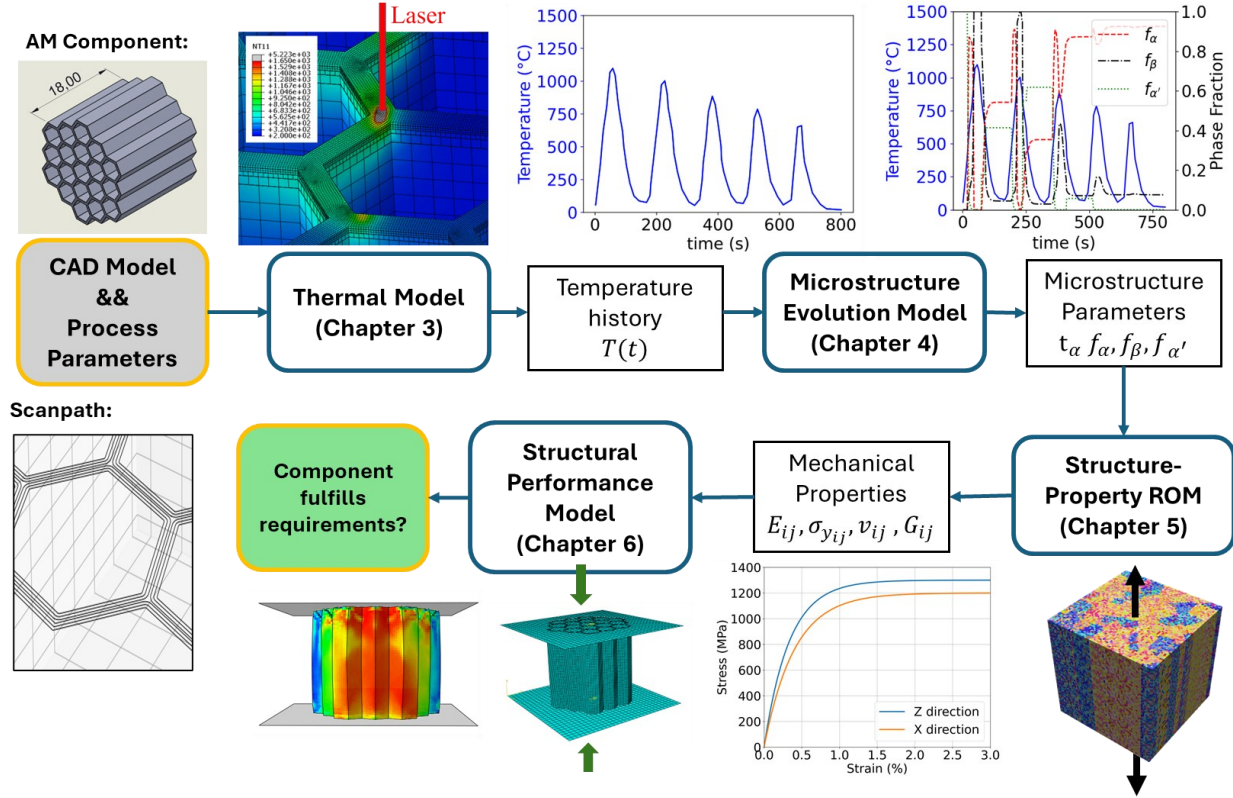


Figure 66. Schematic representation of the developed PSPP framework, showing an example for a 3D printed honeycomb. The diagram illustrates how a structural FEA model with spatially resolved mechanical properties is generated from the input CAD geometry and process parameters. This is achieved through a thermal FEA model that provides local temperature histories, a microstructure evolution model that predicts the resulting local microstructure, and a crystal plasticity Reduced Order Model (ROM) that determines the corresponding local mechanical properties. (Same as Figure 22, but reused here.)

It should be noted, however, that the transient thermal FEA model employed in the PSPP framework to generate high-resolution thermal histories is computationally intensive. As a result, thermal histories are computed only at a limited number of discrete locations using adaptive time-stepping strategies, as detailed in Chapter 3. Consequently, mechanical properties are also computed only at these discrete points. To extend these results and map the properties across the

entire FEA domain of the structural model, a spatial interpolation scheme is employed, as described in the following subsection.

Therefore, an additional input required by the PSPP model is the specification of spatial locations, referred to as points of interest, at which property calculations are carried out using the PSP framework. The number and spatial distribution of these points can critically influence both the computational cost and the accuracy of the final structural performance predictions. This requirement represents a notable limitation of the current PSPP implementation, as it prevents the model from being fully automated based solely on geometry and process parameters. Instead, expert knowledge in materials science and additive manufacturing is needed to appropriately select the points of interest for interpolation, decreasing its utility. The author acknowledges this constraint and expresses the expectation that it may be addressed in the future through the development of more computationally efficient thermal models for PBF processes. If the computational demands of the thermal model are mitigated, it would be feasible to determine the material properties throughout the entire component with high spatial resolution. This is because both the microstructure evolution model and the structure-property model are sufficiently fast to compute material properties at a large number of spatial locations, provided that the corresponding thermal histories are available.

6.1.1 Local Property Assignment with Spatial Interpolation

Due to the substantial computational expense of the thermal model, high-resolution thermal histories required for microstructure evolution can only be computed at a limited number of discrete spatial locations. As a result, microstructural evolution and the corresponding mechanical properties are evaluated exclusively at these selected points. To enable the assignment of mechanical properties throughout the finite element mesh used in the structural performance simulation, a spatial interpolation procedure is introduced.

In this approach, each separate material property ($E, \nu, \sigma_y \dots$) is treated as an independent scalar quantity, which is interpolated in three-dimensional space based on its known values at the designated points of interest. Therefore, the spatial interpolation does not consider any relationship between the properties. Specifically, the interpolation is performed at the centroid of each element in the structural FEA mesh for all material properties considered in the model. The procedure is illustrated in Figure 67, using a simplified example of a cube with known yield strength values at

eight discrete internal points. The known material properties at these points would be yielded by the PSP model at the points of interest. The element centroids are read through a Python script using the API from Abaqus. Subsequently, to incorporate spatially varying mechanical properties into the Abaqus simulation, each element is assigned a material definition corresponding to the interpolated properties at its centroid, as shown in Figure 57.c). This was done through the main Python framework, which performed the automatic creation of an element set and section assignment for each element in the mesh and wrote the final Abaqus .inp file. Finally, it can be seen in the example simulation of Figure 57.d) how this has the expected effect on the stress values computed in the FEA model, which show a gradient in stress equivalent to the yield stress differences in the known points.

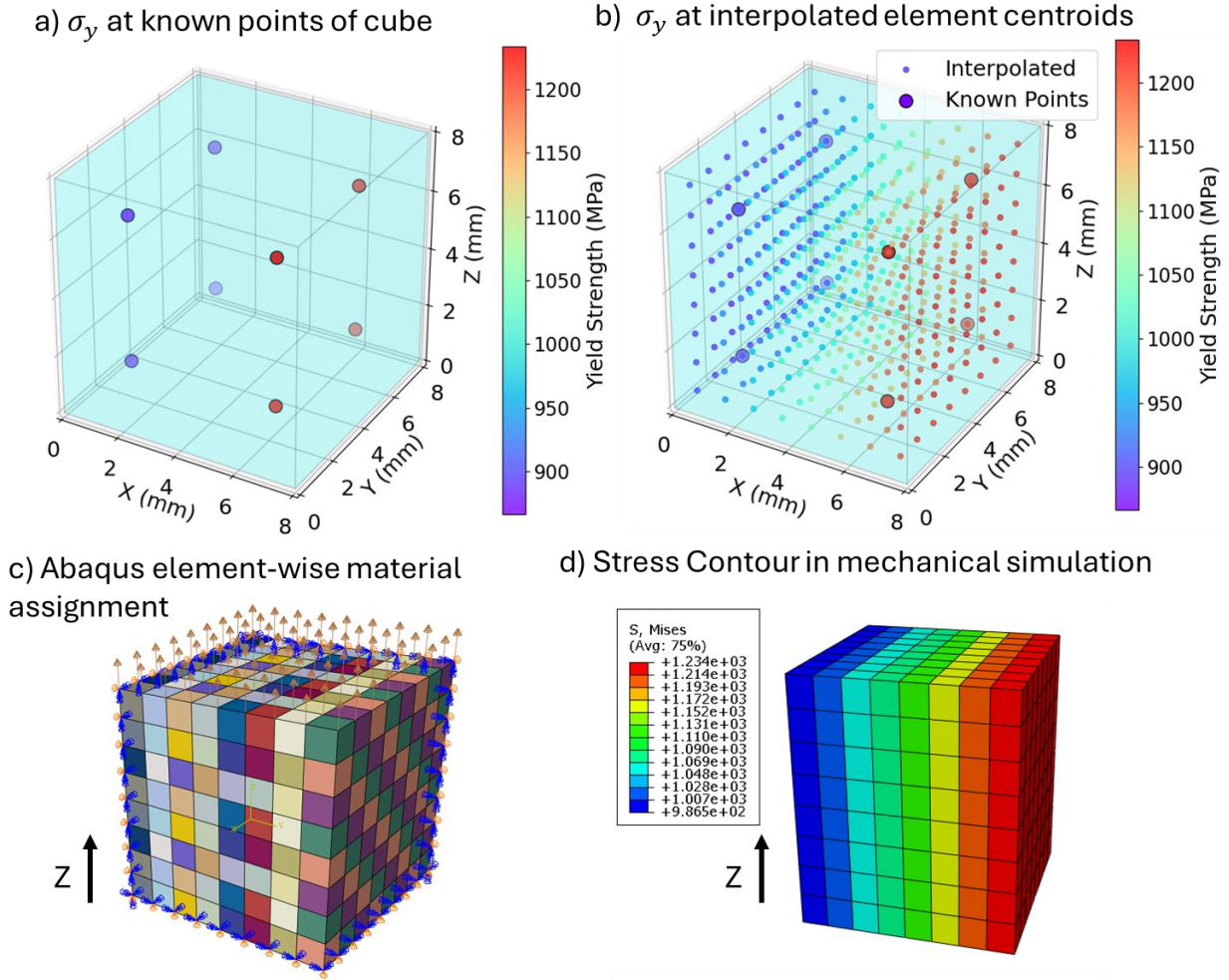


Figure 67. Illustration of the local property assignment procedure developed for the PSPP model using a simplified cube example. In **a)**, the cube contains eight discrete internal points where the yield strength is known. These values, which exhibit a higher yield strength on the right side compared to the left, would be what is computed by the PSPP model at the selected points of interest. **b)** The interpolated yield strength values at all element centroids within the cube's Abaqus mesh shown in **c)** and **d)**. **c)** Element-wise material assignment in Abaqus, where each element has different material properties computed with the spatial interpolation. This is visually represented in Abaqus by varying the colours of the elements, where each material is assigned a different colour, and it shows that each element has been assigned its own material properties. **d)** Result of a mechanical simulation using the assigned local properties, where a smooth stress gradient from left to right is observed, reflecting the spatial variation in yield strength.

While this element-level interpolation offers a practical implementation, a theoretically more accurate alternative would involve performing the interpolation at the level of the integration points. This would result in a smoother spatial variation of material properties and, consequently, a more continuous mechanical response. However, such an implementation in Abaqus requires the

use of a user-defined material subroutine (UMAT), which significantly increases the complexity of the workflow. Nonetheless, the author highlights this approach as a potential enhancement to the current model. Conversely, in cases where the structural model contains a large number of elements, the data volume associated with assigning element-wise material properties could be reduced by grouping elements into clusters or element sets. Each cluster can then be assigned the interpolated properties corresponding to a single representative interpolation point in the geometrical centroid of the cluster.

With respect to the specific interpolation methods, several alternatives are available. A comparison between two common spatial interpolation methods is displayed in Figure 68. These are Radial Basis Function (RBF) interpolation and extrapolation, and linear interpolation with nearest-neighbour fall-back extrapolation. In this work, the former approach was chosen, RBF interpolation, implemented via the scikit-learn Python library [205]. However, it must be noted that this method inherently supports extrapolation, which can lead to unreliable predictions in regions far from the interpolation points. This is seen in Figure 68.b), where it can be seen that outside of the geometrical hull of points, higher strength values than those in the known points are seen. Therefore, it is essential to ensure that peripheral areas of the component are adequately covered with points of interest, as extrapolated values in poorly sampled regions may yield non-physical results. An alternative approach is to employ linear interpolation with a nearest-neighbour fallback strategy, which provides more conservative estimates outside the convex hull of the known data points. However, this approach can lead to jumps in the material properties for elements outside of the convex hull of known points, therefore it was not deemed appropriate.

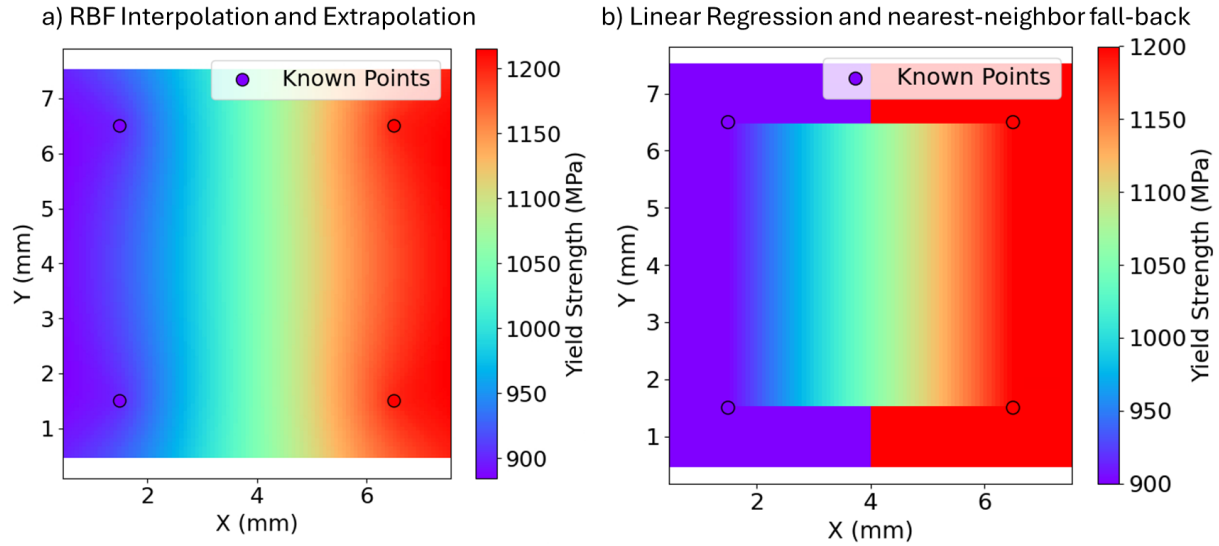


Figure 68. Comparison of two common spatial interpolation schemes. It shows in a contour what would be the interpolated values given 4 known points. **a)** Radial basis function (RBF) interpolation produces a smoothly varying field that naturally extrapolates beyond the convex hull of known points, but it can generate values outside the original data range, resulting in unexpectedly high or low strengths in remote regions. In contrast, piecewise-linear interpolation with nearest-neighbour fallback, shown in **b)**, ensures that all interpolated values remain bounded by the known minima and maxima, offering a more conservative estimate. However, this approach introduces abrupt jumps outside of the hull boundary, which may create non-physical mechanical behaviour.

6.2 Experimental Model Validation Methodology

To validate the PSPP approach, a compression test on an additively manufactured Ti-6Al-4V honeycomb structure was modelled, and the resulting stress-strain curve was compared with experimental data from an equivalent test reported in ref. [216]. The mechanical model of the compression test consisted of an explicit structural FEA simulation utilising local elasto-plastic properties computed through the PSPP model. Both the manufacturing process simulation and the subsequent compression simulation aimed to closely replicate the conditions described in the experimental reference [216], and are explained in the following subsections.

6.2.1 Experimental Methods

The experimental work from Lin et. al. in ref. [216] was used. In this work, honeycombs were built in a LPBF system using the process parameters displayed in Table 12 and then their mechanical performance was analysed through a compression test. The geometry of the honeycombs is

displayed in Figure 69.a), the manufactured honeycomb is displayed in Figure 69.b), and the compression test is shown in Figure 69.c).

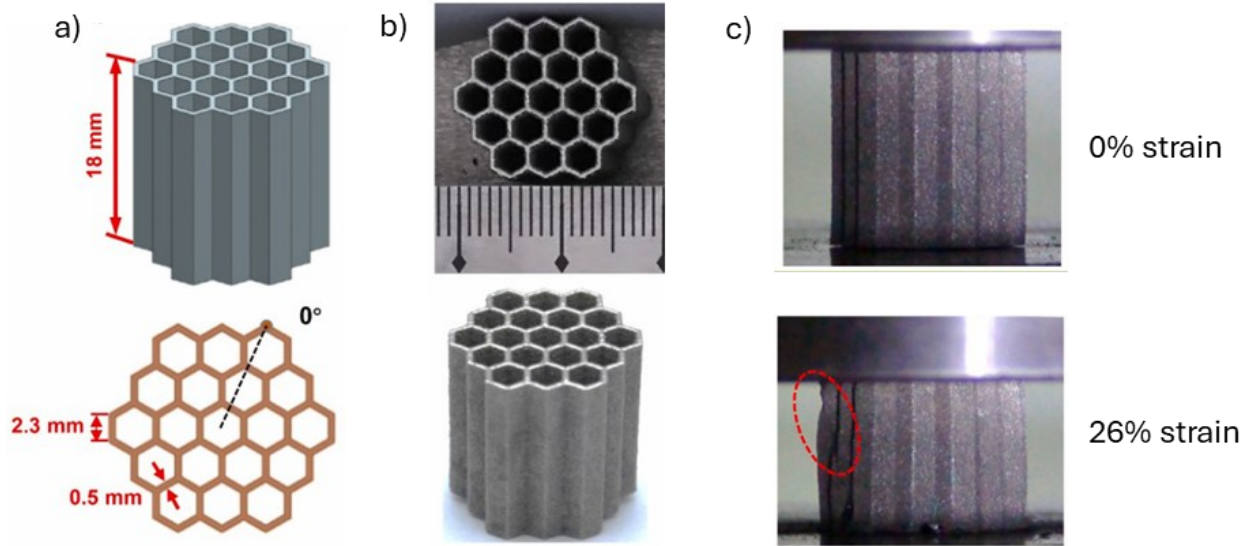


Figure 69. **a)** CAD model and dimensions of the experimentally tested honeycomb that is simulated in this work. These measurements were used to generate the CAD model that is input in the PSPP model. **b)** Images of the additively manufactured honeycomb. **c)** Images of the compression test at different strain values. All images were reproduced from ref. [216].

Table 12. Process parameters used to additively manufacture the experimental Ti-6Al-4V honeycombs in ref. [216]. These process parameters are used in the thermal FEA model of the process.

Baseline Process Parameters	
Scan Speed (v)	800 mm/s
Laser Power (Q)	250 W
Laser Spot Radius (r)	35.0 μm
Layer thickness (t_{layer})	50 μm
Platform Temperature (T_{preheat})	200 °C
Hatch Spacing (h)	80 μm
Scan Strategy	Chessboard

The honeycombs were mechanically tested through uniaxial compression testing with a loading velocity of 1 mm/min. This yields a strain rate of approximately $\dot{\epsilon} = 9 \times 10^{-4} \text{ s}^{-1}$, which is comparable to the strain rate used in the mechanical tests to calibrate the CP models in the structure-property model in **Chapter 5** ($\dot{\epsilon} = 1 \times 10^{-4} \text{ s}^{-1}$), and therefore it should not induce a

significant error. A more detailed description of the experimental procedure can be found in ref. [216].

6.2.2 Process-Structure-Property-Performance Model of the Honeycomb Component

As explained in **6.1 Methodology of PSPP Model of AM Ti-6Al-4V**, the PSPP model inputs consist of the CAD geometry representing the manufactured component, the additive manufacturing process parameters, a set of defined points of interest at which material properties are computed, and the mesh used in the structural performance analysis. The local mechanical properties for the structural model are then assigned by spatial interpolation of the properties calculated at these points of interest.

The CAD model used is displayed in Figure 70.a), which matches the geometry from the experimentally tested honeycombs shown in Figure 69.a). Figure 70.b) shows the points of interest used in the model. Points of interest were chosen at three different heights, two near the bottom and top, and one in the middle. No points were selected directly at the bottom or top because these points have specific thermal phenomena and are not usually representative of the material in the bulk. The points at the very bottom cool down very quickly and the points at the top do not suffer any annealing from being heated by top layers, but since these only happen at a few layers before getting stabilised they do not have a big impact on the overall elasto-plastic compressive behaviour of the whole structure [25].

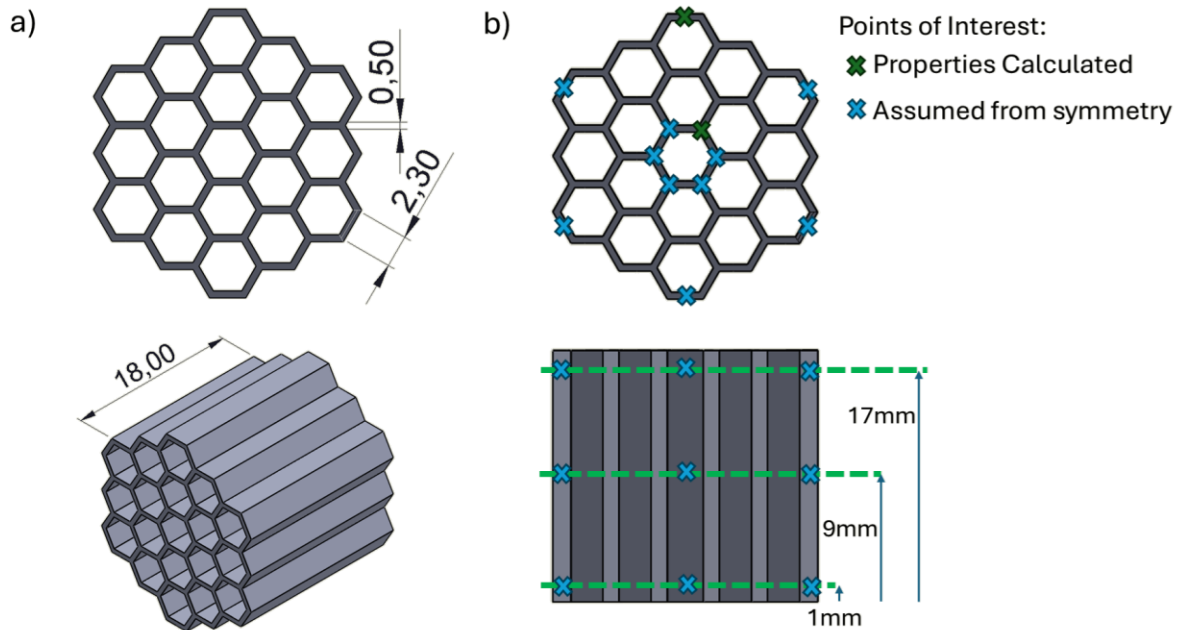


Figure 70. **a)** A CAD model used as input for the PSPP model. **b)** Points of interest defined for the PSPP model. The green points indicate locations where material properties will be calculated using the physical models. By leveraging symmetry, these calculated properties are then assigned also to the equivalent blue points, facilitating spatial interpolation throughout the component. The points shown in the top picture are defined at the three different heights shown in the bottom picture.

At each height, the high-resolution thermal histories and subsequent material properties were only computed at two points, shown with green crosses in Figure 70.b. Then, leveraging the symmetry of the structure, the computed properties were also applied to the equivalent symmetric positions for the spatial interpolation, where the material properties are expected to be similar. This similarity occurs thanks to the usual 67° rotation that is applied in the scanning direction after every layer in AM, reducing directional effects. Using this symmetrical approach in the model considerably reduces the number of points necessary for accurate thermal history computations, thereby significantly decreasing computational expense, while still maintaining sufficient known points for precise spatial interpolation onto the final structural FEA mesh.

For the process parameters, the same parameters as in Table 12 were used, aiming to correctly simulate the experimental AM process. The inter-layer time and FOD, which were not reported in the reference, were assumed to be 12 seconds and 0 mm, respectively. These are the default values in the RenAM 500S machine.

With these inputs defined, as explained in **6.1 Methodology of PSPP Model of AM Ti-6Al-4V**, the PSPP model assigns local elasto-plastic properties to a mesh used for structural performance FEA model. This mesh is detailed in the next subsection, which explains the structural FEA model developed for the compression test of the honeycomb.

6.2.2.1 Structural Performance FEA Model of the Honeycomb Compression

This subsection explains the structural performance FEA model used to reproduce the compression test of the AM honeycombs. The FEA model consists of a dynamic explicit non-linear structural simulation implemented in Abaqus. In this simulation, two rigid plates are positioned above and below the honeycomb structure. Then, the top plate is applied a constant downward velocity of 1 mm/min , coinciding with the experimental compression test. Through contact analysis, this applies a deformation on the deformable honeycomb mesh, which resists it according to its elasto-plastic mechanical properties and applies a reaction force on the rigid plates. The reaction force and displacement in the top rigid plate were requested from Abaqus and used to calculate the simulated stress-strain curve. To calculate the stress, the cross-sectional area was measured from the CAD model with the measurement tool in SolidWorks.

This is computed by solving the governing equations of mechanical equilibrium using the Galerkin method [217]. This approach uses a discretisation of the domain into elements and approximates the displacement field with shape functions, ensuring the weighted residual of the equilibrium equations is minimised. Abaqus internally formulates and solves this nonlinear problem, accounting for the elasto-plastic mechanical behaviour applied to the honeycomb material, while enforcing contact constraints and friction between the deformable mesh and rigid plates. More information about the specific approach can be found in the Abaqus documentation [105].

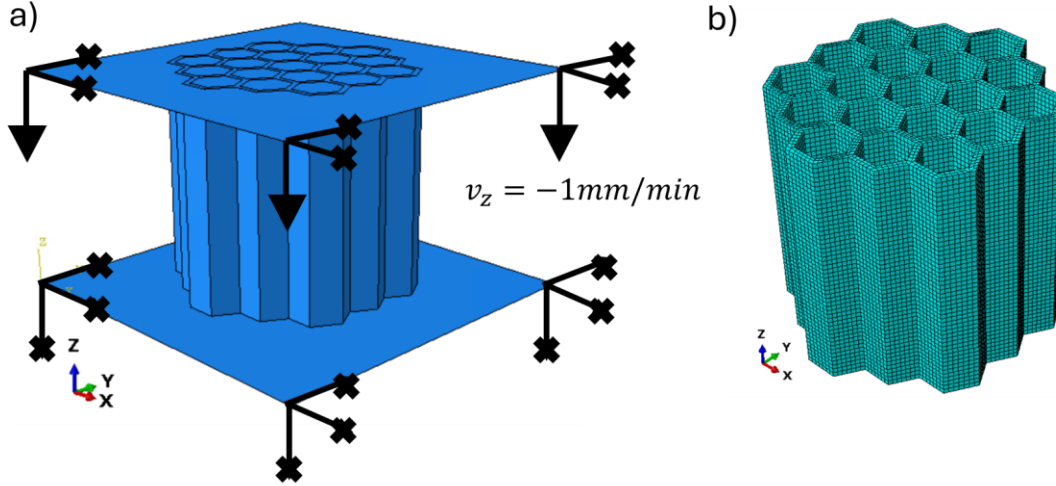


Figure 71. **a)** Schematic of the structural performance FEA model simulating the compression test of the additively manufactured Ti-6Al-4V honeycomb. It shows the two rigid plates and the honeycomb and the boundary conditions applied, which consist of a downward velocity in the top plate while restricting all other movements in both plates. The restricted directions in each rigid plate are marked with crosses. **b)** FEA mesh used in the model for the honeycomb.

A schematic of the developed FEA model and the mesh used are shown in Figure 71. The FEA model was meshed with linear hexahedral elements (C3D8R) with an approximate global size of 0.35 mm , chosen after convergence analysis. The contact was modelled as hard contact with a coefficient of friction of 0.2. The elasto-plastic material properties were applied element-wise as described in the methodology of the PSPP model. Even though not the aim of the thesis, which focused only on elasto-plastic properties, damage evolution was applied to model the fracture that occurs in the experimental compression test. Specifically, spatially homogeneous damage properties with the Johnson-Cook damage criterion were applied, using the constants $d1 = -0.09$, $d2 = 0.25$, $d3 = -0.5$, obtained from ref. [218]. The Abaqus solver automatically handles the physical coupling between this damage evolution and the input plasticity behaviour. Mass scaling was included in the dynamic model with a target time increment of 1 ms , keeping a balance between speed and accuracy, but this mostly influenced the post-fracture behaviour, which is not of high interest for this study.

6.3 Results and Discussion

Figure 72 shows the results from the thermal FEA model of the AM process, which yielded the thermal history in the points of interest defined for the PSPP model. It shows how high-resolution thermal histories were successfully obtained at these points along the entire process by leveraging the adaptive time incrementation strategy explained in **Chapter 3**. These thermal histories were used to calculate the local mechanical properties at these points with the previously described methodology.

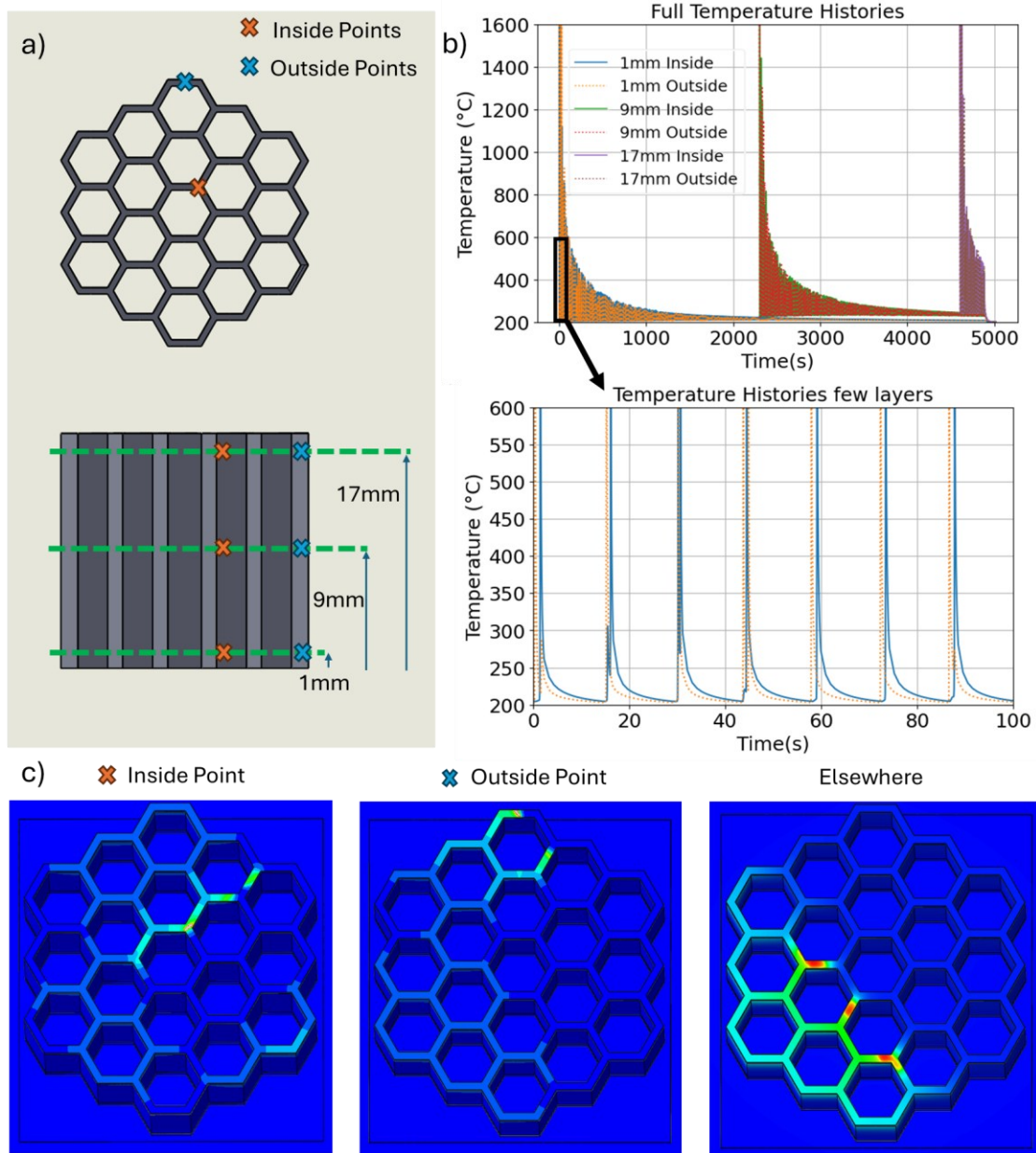


Figure 72. Results from the thermal process model of the experimentally produced honeycomb. **a)** Schematics illustrating the points of interest at which high-resolution thermal histories were computed. They were calculated at one interior and one exterior location across three distinct heights. **b)** Plots of the thermal histories computed. The top plot shows thermal histories computed at all points of interest throughout the entire process, and the bottom plot shows a detailed view of the thermal histories during the deposition of a few layers immediately following the completion of the 1 mm layer, showing the resolution of the thermal history. **c)** Temperature contour fields during the printing of a layer of interest (9 mm). It shows how a fine temporal resolution is used around the points of interest, while coarser time increments are applied elsewhere. The melt pool is shown grey by changing the contour to that colour about the melting temperature of Ti-6Al-4V (1650 °C), showing how it is captured in the points of interest where temperature is being measured.

Figure 73 visualises the microstructure and mechanical properties along the component computed with the PSPP model by applying the microstructure evolution model and the structure-property model on the temperature histories from Figure 72. By leveraging the symmetry of the honeycomb structure, the computed properties were extended to equivalent points and then interpolated across the entire mesh that is used in the structural FEA model of the compression test. Specifically, Figure 73 shows the final martensite phase fraction ($f_{\alpha'}$) and the yield stress in the Z direction at 3.5% strain, which was one of the material properties more sensitive to microstructural changes.

Overall, the model did not predict a very significant change of properties across the structure, with a maximum variation of around 30 MPa in yield stress. The yield strength predicted had a close correlation to the amount of martensite predicted in the microstructure, as expected. The bottom of the structure shows the highest yield strength. This can be attributed to higher cooling rates near the substrate, which conducts heat away, and would increase martensite formation. Furthermore, the inside of the structure shows lower yield strength than the outside. This may be explained by higher overheating at the centre of the structure, which would decrease martensite. A higher cooling can also be appreciated for the outside points in the high-resolution thermal histories of Figure 72.b). These are typical thermal phenomena in laser powder bed fusion [219]. These predictions agree with what was reported in the microstructural analysis of the honeycombs in ref. [217], which showed a low variation in microstructure along the honeycomb structure.

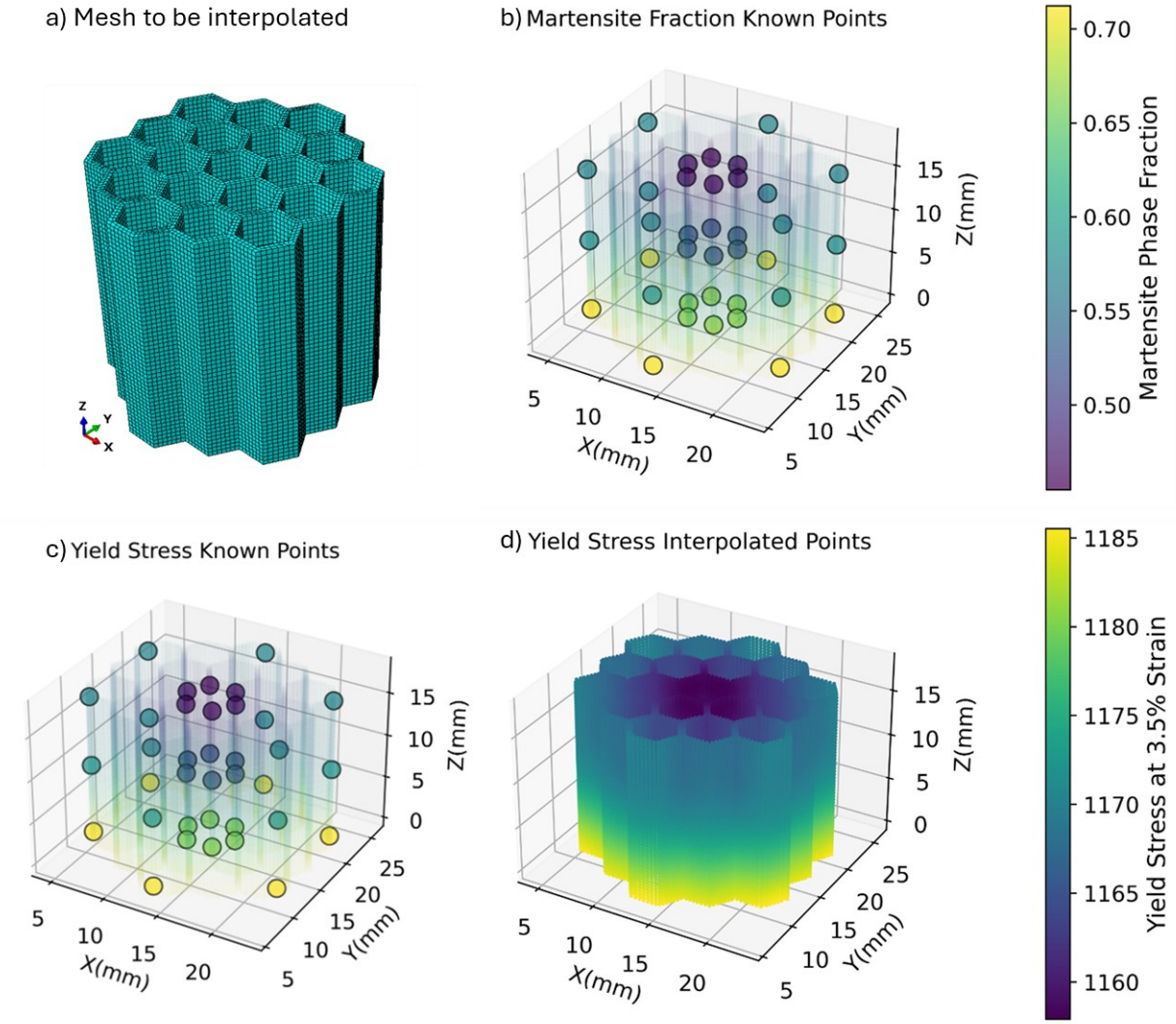


Figure 73. Visualisation of the results of the computation of local mechanical properties for the experimentally produced honeycomb. **a)** Mesh for which the properties have been computed at each element. **b)** Phase fraction of martensite ($f_{\alpha'}$) predicted at each point of interest. **c)** Yield stress in the Z direction at 3.5% strain predicted at each point of interest. **d)** Same yield stress computed at each element centroid after spatial interpolation.

Finally, the results of the structural FEA model using the previously discussed local mechanical properties are displayed in Figure 74. It shows how the simulated compression stress-strain curve compares to its experimental equivalent. When comparing the PSPP stress-strain curve to the experimental one, there are significant differences.

Firstly, the behaviour post Ultimate Tensile Strength (UTS) deviates significantly. The simulated curve has a much more abrupt failure, quickly dropping after UTS. This is related to the

damage properties and the behaviour post-fracture, since the failure mode was cracking and not buckling. Therefore, predicting this correctly would require a high-fidelity model of damage initiation and crack propagation, which is beyond the capabilities of the developed structural model and the overall objective of this study, aimed at predicting elasto-plastic properties.

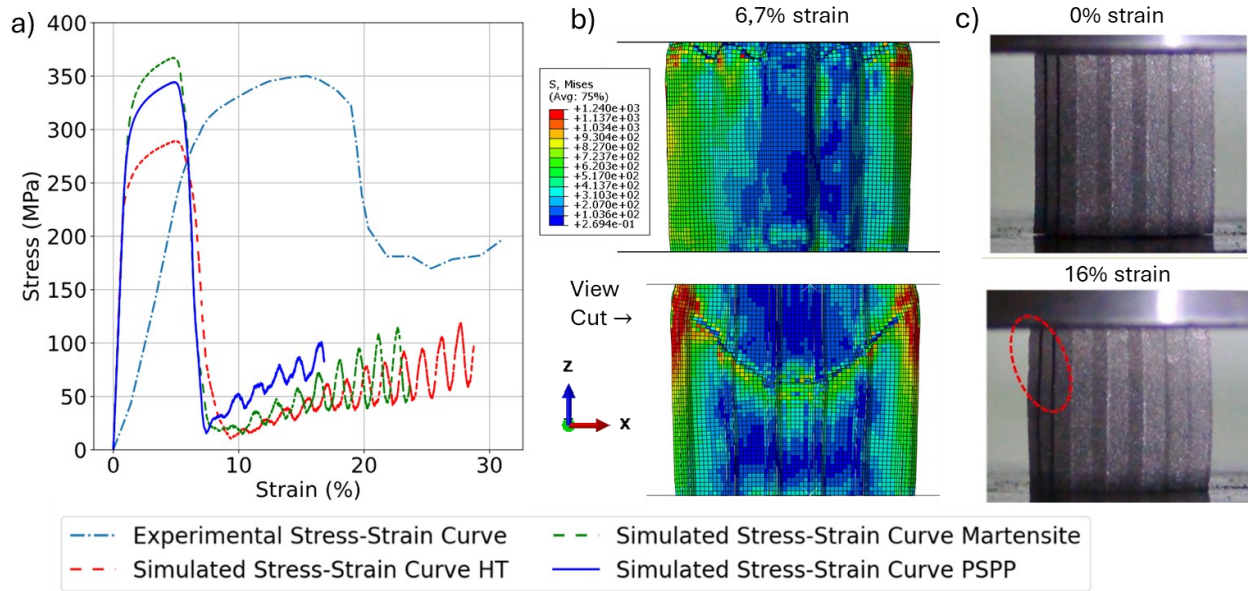


Figure 74. **a)** Comparison between experimentally measured and simulated stress-strain curves for the compression test of the additively manufactured Ti-6Al-4V honeycomb. The simulated curves were computed using the performance FEA model. Three simulated curves were generated: one using material properties predicted by the PSPP model, and two representing extreme microstructural cases, a fully martensitic microstructure ($f_{\alpha'} = 100\%$) and a fully heat treated (HT) microstructure ($f_{\alpha} = 93\%$, $f_{\beta} = 7\%$, $t_{\alpha} = 1.3\mu\text{m}$). These extremes encompass the range of properties that the PSPP model can predict. The data for the experimental curve was extracted from ref. [216]. **b)** Stress contours of the performance FEA simulation short after fracture. It shows a side view, and a view cut such that the failure mode predicted can be easily seen. **c)** Pictures of the experimental compression test at two different strains. It shows that the component is slightly bent before the compression. The region where cracking started is marked in red. These pictures were reproduced from ref. [216].

Regarding the stress-strain behaviour prior to UTS, there is a significant difference in the stiffness between the simulations and the experiment. This could be attributed to the distortion produced by residual stress on the geometry of the tested honeycomb. It is known that significant residual stress can occur in 3D printed Ti-6Al-4V. When a printed component is removed from the build plate, the residual stress can induce significant distortion, especially if not heat treated

like in the case of the experimental honeycomb from ref. [217]. This distortion could mean that in the compression test there would be some compression strain where the honeycomb's top and bottom surfaces are being bent until they are flattened. This would show smaller stress than if there is full contact between the honeycomb's surfaces and the plates since the beginning. Since the simulation models the surfaces to be in full contact since the beginning, it shows a much higher initial stress. Once full contact is made, the mechanical behaviour should be more equivalent between the simulation and the experiment, but this happens at a later strain in the experiment. In order to correctly model this, the distortions would need to be included into the initial geometry in the FEA model, but it has not been done in this work because it would make the property interpolation tedious since they are not predicted in the PSPP model. Introducing residual stress and distortion predictions in the PSPP model would be a significant improvement as seen here, and the author would like to propose it as future work.

Despite these limitations, the model provides reasonably accurate predictions of both yield stress and hardening behaviour. These quantities are expected to converge more closely with the experimental response once the honeycomb reaches full surface contact, and they represent the primary objectives of the PSPP model. This emphasis is particularly relevant since yield stress is the principal parameter typically employed in structural design and topology optimisation.

Furthermore, Figure 74 also displays simulated curves for a case when the honeycomb was assumed homogeneously martensitic ($f_{\alpha'} = 100\%$), and a case where it was assumed heat treated ($f_{\alpha} = 93\%, f_{\beta} = 7\%, t_{\alpha} = 1.3\mu m$), which are the extreme cases of microstructures that the PSPP model could predict. It can be seen here that there could be significantly range of different stress-strain behaviours depending on the properties chosen for Ti-6Al-4V depending on the microstructure, and the PSPP model yielded a reasonable estimate of the yield stress for the printed structure among that range.

Overall, this study shows that it is possible to combine a thermal FEA model, a mean-field microstructure-property model and a reduced order model of crystal plasticity to better estimate the elasto-plastic properties of additively manufactured Ti-6Al-4V and apply them in a mechanical FEA simulation to improve accuracy. However, significant challenges remain for a PSPP model to become industrially relevant. The challenges that are part of the specific models developed have already been described in their dedicated chapters. The discussion in this chapter will focus on the most prominent ones.

The main challenge for PSPP models of L-PBF in the opinion of the author is the computational expense of the thermal FEA process model. Even with adaptive meshing and adaptive time incrementation strategies the thermal FEA simulation took approximately 30 hours to run on 10 cores of Dual Intel Xeon X5650 2.66 GHz CPUs for this small component. It is likely that with more refined adaptive meshing algorithms and a higher CPU count the run-time could be reduced to a few hours and these computational times may be useful to ensure that a final design is not going to fail. However, they make iterative optimisation using this model likely to be unfeasible, which significantly limits the true potential of these models. Therefore, this is one of the first challenges that need to be addressed for PSPP models of AM to become a reality. Some possible solutions may go in the direction of machine learning surrogates [220] or lumped-sum approaches that add the heat form several layers at once [221]. Luckily, the mean-field microstructure evolution model and the reduced-order model used for the structure-property model are fast and do not pose this problem. If the computational expense of the thermal FEA model is solved, it could also avoid the need to define points of interest in the model for interpolation since high-resolution thermal histories could be computed at each integration point. This would simplify the usability and applicability of the model.

Another significant challenge that has not been addressed much in this study is the prediction of fracture. It is likely that PSPP models will also need to predict damage and fatigue properties in order to become truly relevant and not simply elasto-plastic properties. However, this will need to include porosity and surface roughness predictions, since they tend to be the main driver and not just microstructure. Furthermore, both of these would need to be included in the crystal plasticity microstructural models, which is not straightforward, although there has been some progress in these approaches [222, 223].

Finally, as seen in the compression test, residual stress and distortion should be included in the PSPP predictions, as they can significantly affect performance. This should not be overly complex as residual stress prediction in AM is already a common workflow among most relevant commercial FEA software [61, 224], but it could still be a significant amount of work to couple it with the entire workflow. Note that residual stress models could also be made more accurate by using part of the developed models in this work to predict the changes in properties along the residual stress process simulation.

6.4 Conclusions

A Process-Structure-Property-Performance (PSPP) computational model for additively manufactured Ti-6Al-4V has been developed. This model takes as input the CAD geometry and process parameters of a component and produces a structural finite element analysis with locally varying mechanical properties, accounting for the influence of the manufacturing process on the heterogeneous material response.

The model's capabilities have been evaluated by comparing its predictions to the results of a compression test performed on an additively manufactured honeycomb structure. An explicit finite element simulation was carried out in Abaqus, where the local mechanical properties were assigned element-wise based on the model output. When analysing the results, a notable discrepancy was observed between the simulated and experimental stress-strain curves. This was primarily attributed to residual distortion in the experimental specimen, which was not included in the simulation, and to the inaccuracies in damage modelling, which was not the focus of the present work.

Despite these limitations, the model accurately predicted the yield strength and hardening behavior, particularly when compared to the mechanical responses of other microstructures that can occur in additively manufactured Ti-6Al-4V. These results demonstrate that the model effectively predicts the local elasto-plastic behaviour and successfully incorporates it into the structural finite element framework for performance prediction. Therefore, the developed model could be used to assert that a final component design will not plastically yield with higher accuracy than using homogeneous material properties that do not consider the AM process.

However, several challenges still exist that need to be addressed in each of the separate models that were used in the PSPP framework. These are well discussed for each separate model on its dedicated chapter, but the author would like to highlight the following three as the main obstacles that need to be overcome for PSPP models of AM to become industrially relevant:

- Computational expense of the thermal FEA model. Even with the adaptive meshing and time incrementation strategies applied, the thermal FEA model remains too computationally expensive to be used in iterative optimisation processes. Possible solutions could be surrogate models or a smart lumped-sum approach which would apply

the heat of several layers at once. Solving this problem would be a significant leap forward for PSPP models and modeling of AM in general, since temperature is a main driver of microstructural heterogeneity and porosity in AM components. The rest of the model used were much less computationally expensive and could be used in optimisation algorithms.

- Prediction of fatigue and damage properties. The current work has focused on prediction of elasto-plastic properties, which are useful for static analysis; nonetheless, fatigue and damage properties predictions must be eventually added to the model for it to be fully driving the component and manufacturing design process. This is a very complex task since it requires the prediction of surface roughness and porosity, i.e., affecting damage initiation and propagation, and its interactions with the microstructure on the final properties.
- Adding the effect of residual stress and distortions. As seen in the compression test, distortion can have an important effect on structural performance and should be included in the PSPP framework. Including the predicted elasto-plastic properties by the PSPP model during the residual stress calculation could significantly improve its accuracy, but it would require making the predicted properties by the structure-property model temperature-dependent.

7. CONCLUSIONS AND FUTURE WORK

This thesis investigated the feasibility of a fully computational and automated framework to predict the structural performance of additively manufactured components based on their geometrical design and processing parameters, following the Process-Structure-Property-Performance (PSPP) paradigm. To this end, a prototype model was developed that enabled a detailed and practical analysis of the approach. This was done specifically for the titanium alloy Ti-6Al-4V and the Laser Power Bed Fusion (LPBF) AM process, although several of the insights gained are expected to be transferable to other materials and additive manufacturing processes.

The literature review in Chapter 2 showed that it is widely recognised that additive manufacturing of Ti-6Al-4V induces significant defects in the material. Some of the most prominent ones are porosity and surface roughness, which have significant effects on structural performance and fatigue life. Another important one is residual stress and distortion, which can

lead to poor geometrical tolerances and affect structural performance. Microstructural heterogeneity, however, was identified as a critical and often overlooked challenge for understanding property variability and thus became the focus of this work. While a comprehensive PSPP model would ideally encompass all defects, this thesis concentrated on predicting microstructure evolution and its influence on elasto-plastic properties, with subsequent integration into finite element models for structural design.

During the literature review, it was also elucidated that most of AM material defects are closely related to the thermal phenomena that the material experiences during the build. For the microstructure, this did not only include the melting process when the laser melts the powder and welds the material to the bottom layer, but also the continuous heating and cooling cycles that the material experienced when the upper layers are being welded, which produced local annealing effects. This makes the thermal history of a material point in the component not only related to the process parameters input into the additive manufacturing machine, but also the geometry. Therefore, the first step in the PSPP model was the development of a process model that would yield the temperature history along the entire AM process in different regions of the component. This was done through a thermal FEA model that took as input the geometry of the component and the process parameters that are given to the AM machine for printing. The developed model showed decent accuracy in predicting thermal histories close and far from the melt pool when contrasted to experimental results from the literature. However, one of the main drawbacks of the developed thermal model was its high computational expense. Since it must capture the fine resolution of powder melting and solidifying, which happens on the micro-second scale during a manufacturing process that can take several hours or even days, the computation of the entire thermal history took significant time and prohibits using this model in optimisation algorithms. The computational expense for computing thermal histories is one of the main obstacles for PSPP models and thermal management of AM in general, so the author suggests solving this problem as a crucial next step in the development of AM PSPP models. Nonetheless, although it could not be used iteratively due to its computational expense, the developed model could still be used as a last digital check for a given design, being significantly more accurate than conventional models with homogenous properties.

Once temperature history was computed, the next step was to calculate the final microstructure in the component for a given thermal history. This was accomplished through a fast

mean-field analytical microstructure evolution model that computed the phase fractions of α , α' and β and the lath thicknesses. When contrasting with in-house and external experimental measurements from the literature, the model effectively captured the kinetics of microstructure evolution in Ti-6Al-4V during additive manufacturing and could be integrated with thermal FEA models to form process-structure predictions based on geometry and process parameters. This demonstrated the potential for digitalising the microstructure evolution in AM of Ti-6Al-4V, enabling tailored microstructure and mechanical property predictions. Future acceleration of the thermal model could allow automated optimisation of process parameters and geometry for desired outcomes. However, ensuring melt pool stability will require additional coupled models, as process parameter changes to modify the microstructure were seen to cause other manufacturing defects. Also, experimental validation revealed some discrepancies attributed to uncertainties in the thermal model, parameter calibration, and difficulties in microstructure measurement. Developing standardised measurement methods will be crucial. Despite current limitations, the developed model, especially when refined with machine-specific corrections, holds a promise for reliable microstructure prediction and practical applications in process engineering.

Following microstructure prediction, a structure-property model was developed to estimate elasto-plastic properties corresponding to the microstructural features obtained from the microstructure evolution model. This model was constructed based on a reduced-order formulation of crystal plasticity simulations performed on synthetic microstructures, which were generated according to the predicted phase fractions and lath thicknesses. The resulting model yields the orthotropic elastic constants, the Hill-type yield surface and the isotropic hardening curve, for any given combination of phase fractions and lath thicknesses. Therefore, the results can be easily input in most commercial FEA software for structural performance simulations. The model results were contrasted with experimental tensile tests of AM Ti-6Al-4V samples. The results showed good agreement between the predicted tensile test curves and the experimental ones. Some limitations were observed for heat-treated samples where grain-boundary α reduced ductility and strength, a phenomenon not currently included in the models. However, this happens in heat treated samples at very high temperatures for prolonged times, and it is not expected to happen during the AM process, which is the main use-case for this model. Nonetheless, it would be a positive addition to add the prediction of grain boundary α and its effects to the microstructure evolution and the structure-property models. An interesting find about the developed structure-property model is that,

thanks to the reduced-order model, the properties for a given microstructure could be calculated almost instantly, instead of the several hours needed to compute the full-field CP model.

Finally, the process, structure, and property models were combined into a PSPP framework for structural performance prediction. The workflow generated location-specific elasto-plastic properties at selected points, which were mapped onto the remaining FEA mesh through spatial interpolation. This produced a structural FEA model of the AM component with local mechanical properties that can be used in an arbitrary structural simulation to assert if it will perform as expected. A significant drawback of the current developed model is that it requires to manually select the points in the component where the properties will be calculated with the previous models. This occurs because the thermal model is too expensive to yield the thermal history needed along all the elements of the FE mesh, requiring reducing the points of calculation and spatially interpolate the results. Reducing the expense of the thermal model could remove this drawback. The accuracy of the developed PSPP model was contrasted with a compression test of an additively manufactured honeycomb, which showed good agreement when contrasting the yield strength and hardening. However, there were significant deviations in the predicted stiffness, which were attributed to the distortions from residual stress not being included in the FEA model. Adding the prediction of residual stress and distortions to the PSPP model would be a significant step forward. Likewise, adding the prediction of damage and fracture would significantly expand its applicability.

7.1 Summary of Key Contributions

In summary, this work demonstrated the potential of a digital PSPP approach for additive manufacturing by:

- Developing a thermal model of PBF that links process parameters and geometry to local temperature histories along the entire process.
- Implementing a microstructure evolution model that predicts phase transformations and lath thicknesses with reasonable accuracy.
- Establishing a reduced-order structure-property model capable of near-instant prediction of anisotropic elasto-plastic behaviour.
- Integrating these models into a structural performance simulation framework validated against experimental structural tests.

Although computational expense and model scope remain limiting factors, the research provides a solid foundation for digital design and performance assessment of AM components. Future developments should focus on accelerating thermal simulations, incorporating residual stress and damage models, and improving experimental validation/calibration standards. With these advances, PSPP frameworks could enable predictive, automated, and optimised design of additively manufactured structures.

7.2 Summary of Possible Next Steps

The author would like to suggest the following topics as possible research that could advance the PSPP modelling of the AM processes and therefore its industrial applicability. These have been discussed in detail along the thesis but have been gathered in this subsection for better readability.

- Acceleration of thermal AM models for predicting microstructure.
- Combination of thermal AM models and microstructure evolution models with optimisation frameworks to ensure microstructural homogeneity.
- Prediction of the texture and morphology of parent β grains with thermal models and cellular automaton methods, and include the results in CP structure-property models.
- Predicting grain boundary α and applying it in structure-property models.
- Predicting residual stress and distortions and apply them in component-scale structural FEA models.
- Predicting damage with CP structure-property models and apply it the component-scale structural FEA models.

APPENDIX A. OPEN-SOURCE CODE REPOSITORIES

This appendix contains links to different repositories with the software frameworks developed and used throughout the thesis.

1. Refined_Thermal_FEA_Additive

A Python library to perform high resolution thermal modelling of PBF processes with Abaqus. It includes adaptive remeshing and time incrementation, drastically reducing computational expense. It yields the thermal histories at the points specified by the user for the entire process.

Link: https://github.com/lreighbua/Refined_Thermal_FEA_Additive

2. Analytical_Phase_Transf_AMTi64

A Python library to calculate microstructural parameters in Ti-6Al-4V during PBF for a given thermal history.

Link: https://github.com/lreighbua/Analytical_Phase_Transf_AMTi64

3. CP_Parameter_Calibration_w_surrogate_optimization

An optimization tool written in matlab to automatically fit material parameters to experimental stress-strain curves for phenomenological CP models in Damask.

Link: https://github.com/lreighbua/CP_Parameter_Calibration_w_surrogate_optimization

4. Generate_Ti64_PBF_Property_Database_with_Damask

Code to generate a structure-property database using Damask CP simulations relating phase fractions and lath thicknesses to tensile properties for PBF Ti-6Al-4V.

Link:

https://github.com/lreighbua/Generate_Ti64_PBF_Property_Database_with_Damask

5. Ti64AM_structure_property_ROM

Structure-property ROM for PBF Ti-6Al-4V that instantly yields elasto-plastic material properties for a given set of microstructural parameters.

Link: https://github.com/lreighbua/Ti64AM_structure_property_ROM

6. Process_Structure_Property_Performance_Model_Ti64_PBF

A simulation framework for PSPP modelling of PBF Ti-6Al-4V. It generates an Abaqus input file of a component with local elasto-plastic mechanical properties that can be used for arbitrary FEA simulations of structural performance.

Link:

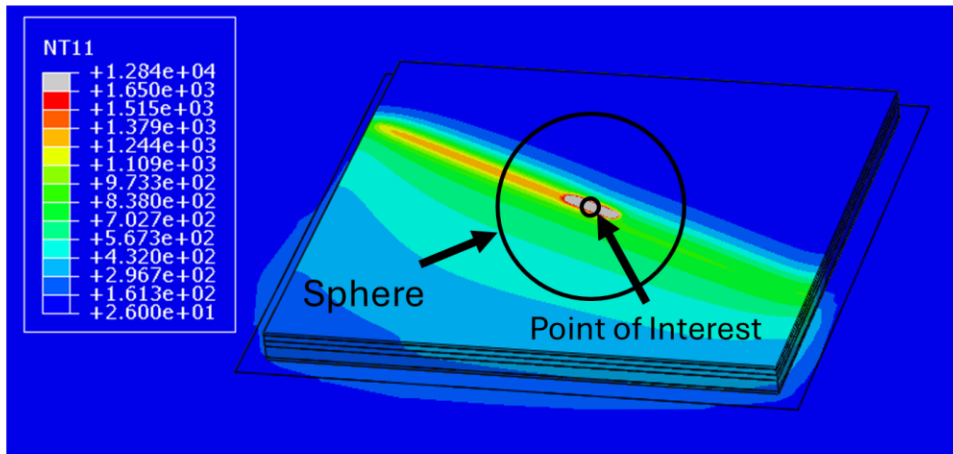
https://github.com/lreighbua/Process_Structure_Property_Performance_Model_Ti64_PBF

APPENDIX B. THERMAL FEA MODEL ADAPTIVE TIME INCREMENTATION ANALYSIS

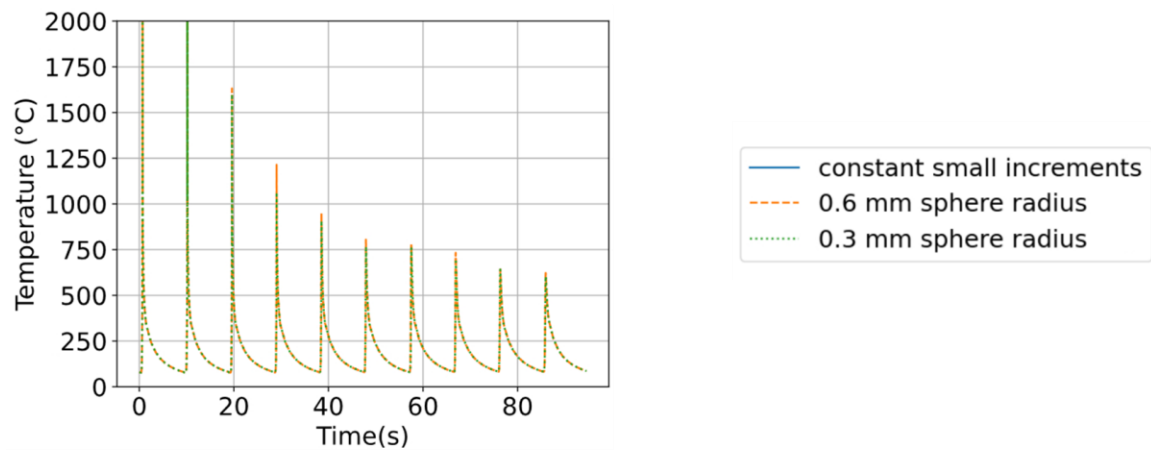
The adaptive time-incrementation strategy used in the thermal FEA model makes possible to obtain high resolution thermal histories at selected points at a much lower computational cost, but its accuracy compared to a constant short time step will depend on the size of the sphere of interest that is used. In order to analyse this, the additive manufacturing of a $10\text{mm} \times 10\text{mm}$ square has been simulated with different sizes of the sphere of interest, as shown in Figure 75.a). The time increment outside of the sphere of interest is set to 60 ms , and to 1 ms inside.

In Figure 75.b), the temperature histories obtained using two different spheres of interest with radii of 0.3 mm and 0.6 mm radius are compared. It is seen that for the radii values that were analysed, sphere of interest size slightly affects the maximum temperatures obtained at the peaks, but the cooling rates remain very similar, as well as the residual heating of the structure. This difference should not affect significantly microstructure evolution since these peaks happen over a very short period of time. In Figure 75.c), a similar comparison can be seen between the case with a sphere of interest of radius 0.6 mm and a case where no adaptive time incrementation is used, applying a constant time incrementation of 1 ms , which is the same one that is applied when the laser is scanning inside the sphere of interest. Here, very small differences can be appreciated as well. However, when zooming into one of the peaks, as shown in Figure 75.d), the differences in time-resolution become apparent. Nonetheless, the magnitude of temperature changes slightly and during short times, which should not affect significantly microstructure evolution.

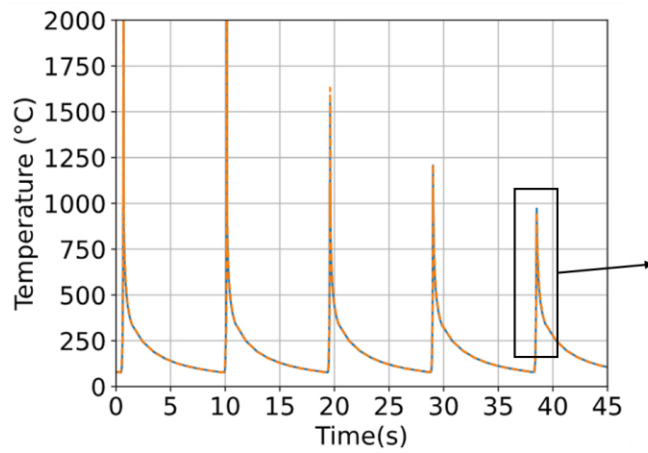
a) Field Output of the simulation



b) 0.6 mm vs 0.3 mm sphere of interest radius



c) 0.6 mm sphere of interest radius vs no sphere



d) Single peak zoom-in all 3 cases

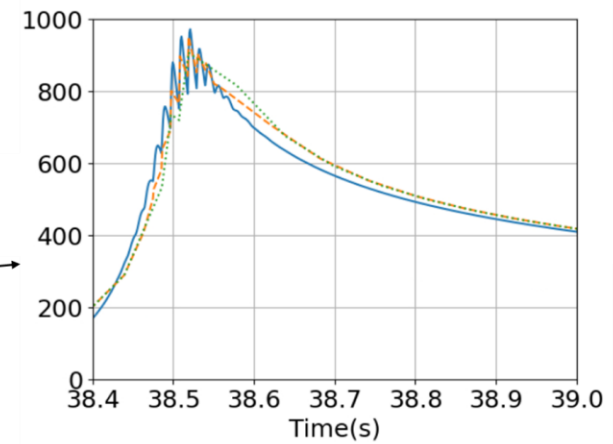


Figure 75. Analysis of the effect of the size of the sphere of interest in the computed temperature time histories. The figure shows a field output of the simulation used and the temperature histories computed using spheres of different radius, and also a case where a constant small-time incrementation is used instead of adaptive time incrementation. **a)** Simulation field output of powder bed fusion of a 10 mm cuboid used for the adaptive time incrementation analysis. **b)** Comparison of temperature histories for a sphere with a radius of 0.6 mm and a radius of 0.3 mm, showing very similar temperature histories. **c)** Comparison between a sphere of interest with radius of 0.6 mm and a simulation that uses a constant small time incrementation of 1 ms, i.e. no adaptive time incrementation is used, and it shows similar results as with time incrementation. **d)** A plot showing a single peak, where differences in the resolution can be appreciated.

The effect of the size of the sphere on the predicted microstructure evolution is shown in Figure 76, comparing using a radius of 0.3 mm against a larger and more accurate radius of 0.6 mm. As it can be seen, the predicted microstructures at the end are similar, with differences below the margin of error expected for this kind of models.

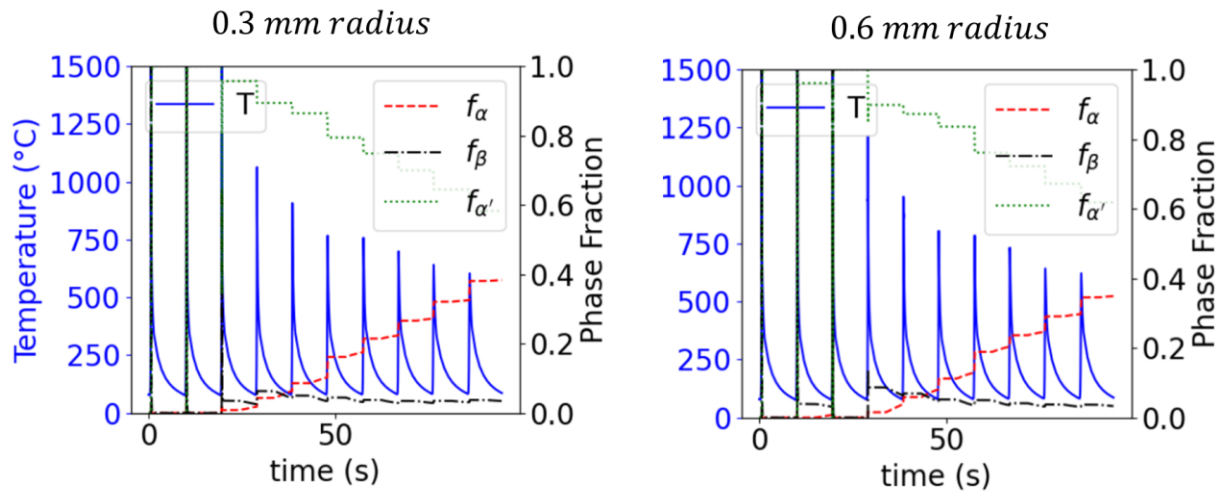


Figure 76. Effect of the size of the sphere of interest on the predicted microstructure evolution. It shows the phase fractions predicted during printing using radii of 0.3 mm and 0.6 mm for the sphere of interest.

Based on this analysis, it can be seen that using a sphere of interest of 0.3 mm yields very similar microstructure evolution and time history results as using a constant short time increment. Therefore, for the rest of the thermal simulations in this work, a radius of 0.3mm has been used, since it is shown to offer a good balance between accuracy and computational expense. However, the author acknowledges that a deeper analysis and optimization of the time incrementation parameters could improve the accuracy and efficiency of the approach.

APPENDIX C. THERMAL FEA MODEL MESH SENSITIVITY ANALYSIS

Throughout this thesis, the thermal FEA models employ hexahedral elements with a minimum side length equal to the layer thickness, which is predominantly $60\ \mu m$. To assess mesh sensitivity, the following analysis examines the impact on the thermal history and temperature fields when the mesh is refined by a factor of two for a $10\ mm$ cube with a layer thickness of $60\ \mu m$. The results of the comparison are presented in Figure 77.

The results demonstrate that while further mesh refinement alters peak temperatures and causes slight variations in the thermal field, the thermal history within the temperature range critical for microstructure evolution ($T < 1650\ ^\circ C$) remains largely consistent. Consequently, although potential inaccuracies in melt pool estimation are non-negligible, they are unlikely to propagate into the results of the microstructure evolution model. The selected element size is therefore deemed appropriate for the scope of this research. Nevertheless, further optimization of the meshing strategy could enhance both the computational efficiency and overall fidelity of the model in future applications. Furthermore, the optimal level of mesh refinement is highly dependent on the chosen printing parameters, as these directly influence thermal gradients and melt pool dimensions.

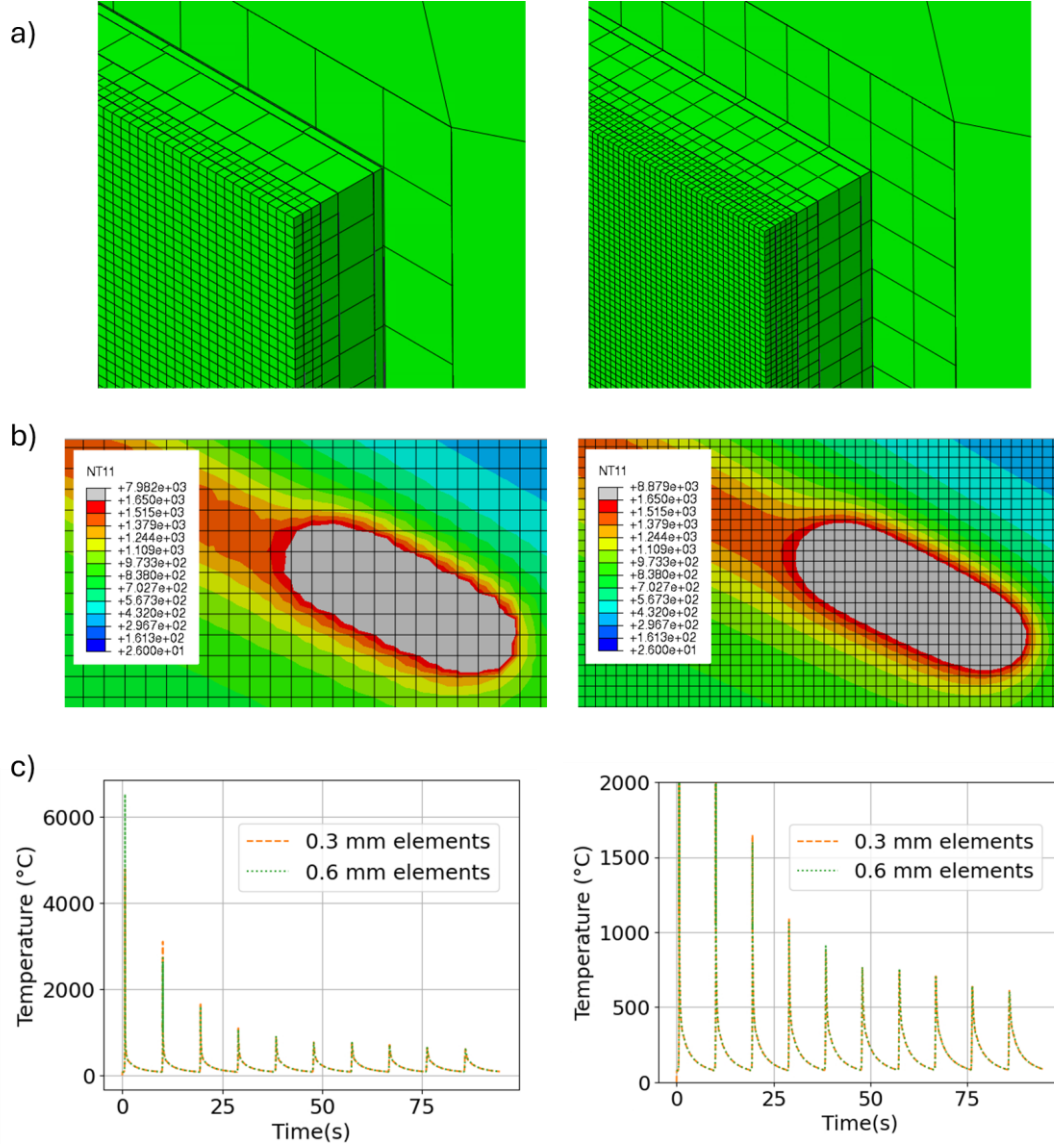


Figure 77. Mesh sensitivity analysis for the thermal FEA model of a 10 mm additively manufactured cube. The standard mesh used in this thesis (minimum element side length of $0.6 \mu\text{m}$, corresponding to the layer thickness) is compared against a refined mesh (minimum side length of $0.3 \mu\text{m}$). **a)** Mesh topologies at the corner of the 10th layer. **b)** Nodal temperature fields around the melt pool at the centre of layer 10 for both mesh densities. **c)** Temperature histories for both mesh densities at the centre of the 10th layer during the deposition of 10 layers, displayed with two different temperature axis limits. While peak temperature predictions vary between the meshes, predictions below the melting temperature ($T = 1650 \text{ }^{\circ}\text{C}$) show no significant variability.

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