

**MULTI-SCALE MULTI-PHYSICS FEM-BASED MODELLING
STRATEGIES FOR METAL ADDITIVE MANUFACTURING
PROCESSES**

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*Dedicated to my inseparable companions,
my parents*

ما زنده به آنیم که آرام نگیریم

موجیم که آسودگی ما عدم ماست!

صائب تبریزی

We are alive because of not to stay,

We are waves, so our stagnation is our death!

-Saeb-e-Tabrizi

1592-1677

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List of Publications

Paper 1

Erfan Azinpour, **Roya Darabi**, Jose Cesar de Sa, Abel Santos, Josef Hodek, Jan Dzugan, Fracture analysis in **directed** energy deposition (DED) manufactured 316L stainless steel using a phase-field approach, **Finite Elements in Analysis and Design**, Elsevier, Volume 177, Pages 103-117, 2020.

Paper 2

Roya Darabi, Erfan Azinpour, Jose Cesar de Sa, Margarida Machado, Ana Rosanete Reis, Josef Hodek, Jan Dzugan, Fracture Prediction Based on Evaluation of Initial Porosity Induced By Direct Energy Deposition, **European Journal of Computational Mechanics**, 29(3):223-254, 2021.

Paper 3

Roya Darabi, Erfan Azinpour, Felipe K Fiorentin, Manuel J Abarca, Jose Cesar de Sa´ and Jan Dzugan, Experimental and computational analysis of additively manufactured tensile specimens: Assessment of localized-cooling rate and ductile fracture using the Gurson–Tvergaard–Needleman damage model, Proceedings of the Institution of Mechanical Engineers Part L Journal of Materials Design and Applications, **SAGE**, 235(6), 1430–1442, 2021.

Paper 4

André A. Ferreira, **Roya Darabi**, João P. Sousa, João M. Cruz, Ana R. Reis and Manuel F. Vieira, Optimization of Direct Laser Deposition of a Martensitic Steel Powder (Metco 42C) on 42CrMo4 Steel, Metals - Open Access Metallurgy Journal, **MDPI**, 11(4), 2021

Paper 5

Roya Darabi, André Ferreira, Erfan Azinpour, Jose Cesar de Sa, Ana Reis, Thermal study of a cladding layer of Inconel 625 in Directed Energy Deposition (DED) process using a phase-field model, The International Journal of Advanced Manufacturing Technology, **Springer**, 119:3975–3993, 2022

Paper 6

Roya Darabi, Erfan Azinpour, Andre Ferreira, Jose Cesar de Sa, Ana Reis, Jan Dzugan, Damage Evolution Simulations via a Coupled Crystal Plasticity and Cohesive Zone Model for Additively Manufactured Austenitic SS 316L DED Components, Metals, Computational Mechanics of Fatigue and Fracture in Metallic Materials, **MDPI**, 12(7), 1096, 2022

Paper 7

Manuel Jimenez Abarca, **Roya Darabi**, Jose Cesar de Sa, Marco Parente, Ana Reis, Multi-scale modeling for prediction of residual stress and distortion inTi–6Al–4V semi-circular thin-walled parts additively manufactured by laserpowder bed fusion (LPBF), Thin-Walled Structures, **Elsevier**, Volume 182, Part A, 110-151, 2023

Paper 8

Joao Sousa, **Roya Darabi**, Ana Reis, Jose Cesar de Sa, Marco Parente Luís Paulo Reis Jose Cesar de Sa, “An Adaptive Thermal Finite Element Simulation of Direct Energy Deposition with Reinforcement Learning: A Conceptual Framework”, Journal of Manufacturing Science and Engineering, **ASME**, 2022

Paper 9

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Paper 11

Roya Darabi, Erfan Azinpour, Ana Reis, Jose Cesar de Sa, Multi-Scale Multi-Physics Phase-Field Coupled Thermo-Mechanical Approach for Modeling of Powder Bed Fusion Process, **Applied Mathematical Modeling**

Paper 12

Joao Sousa, **Roya Darabi**, Amanda Sousa, Ana Reis, Jose Cesar de Sa, Luís Paulo Reis Jose Cesar de Sa, Enhancing Sample Efficiency for Temperature Control in DED With Reinforcement Learning and Moose Framework, Journal of Manufacturing Science and Engineering, **ASME**, 2023

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Abbreviations

Integrated Computational Materials Engineering	ICME
Additive Manufacturing	AM
Metallic Additive Manufacturing	MAM
Three-Dimensional	3D
Computer-Aided Design	CAD
Computer-Aided Manufacturing	CAM
Manufacturing Operations Management	MOM
Computer Numerical Control	CNC
Stereolithography	STL
Powder Bed Fusion	PBF
Directed Energy Deposition	DED
Electron Beam Melting	EBM
Wire Arc Additive Manufacture	WAAM
Laser Engineered Net Shaping	LENS
Directed Light Fabrication	DLF
Laser Solid Forming	LSF
Fused Deposition Modelling	FDM
Light Optical Microscopy	LOM
Scanning Electron Microscopy	SEM
Electron Back-Scattered Diffraction	EBSD
X-Ray Computed Tomography	X-CT
Finite Element Method	FEM
Johnson Mehl Avrami	JMA
Discrete Element Method	DEM
Dynamic Mesh Refinement	DMR
Level-Set Method	LSM
Volume of Fluid	VOF
Finite Cell Method	FCM
Dissipative Particle Dynamics	DPD
Smoothed Particle Hydrodynamics	SPH

Apparent Capacity	AC
Phase Field	PF
Multiphysics Object-Oriented Simulation Environment	MOOSE
Adaptive mesh refinement	AMR
Heat Integration	HI
Neural Network	NN
Artificial Intelligence	AI
Proximal Policy Optimization	PPO
Reinforcement Learning	RL

Abstract

This study encompasses various computational aspects of process modeling in additive manufacturing (AM) with a particular focus on dissipative phase field modeling to predict thermal, mechanical, and microstructural responses. The increasing interest in AM stems from its advanced manufacturing possibilities; however, a comprehensive understanding of defect formation and constitutive/structural responses remains elusive due to the complex multi-physics nature of the process. To address these challenges, a reliable computational approach that considers the multi-scale and multi-physics aspects of AM is required. Advanced numerical techniques have recently emerged, enabling the prediction of defects based on process parameters and facilitating the determination of optimal processing windows for desired mechanical properties. Numerical simulations have proven to be robust, cost-effective, and reliable tools for predicting component quality in AM. In this context, this study aims to propose a process model framework that integrates insights from integrated computational materials engineering (ICME) into AM processes. The study employs two approaches. The first approach couples a thermodynamically consistent phase field model with a transient heat transfer model to track material phase states. This approach divides the domain into state regions separated by a diffusive interface. The phase field variable, obtained from explicit solutions of the Wang phase field formulation, accurately captures the degree of consolidation between the powder and molten phases. An enthalpy-based model is incorporated to handle the nonlinearity resulting from coupling the two approaches. The feasibility of studying melt pool behavior is demonstrated through finite element simulations of a material layer processing using the ABAQUS framework. The simulations are then extended to a multi-layer scale, allowing for the modeling of complex geometries and real-world size patterns. By considering phase field-dependent material properties and leveraging thermal responses, the energy dissipative inequality equation enables the prediction of residual stress and deformations. To explore the influence of laser scanning patterns on structural deformations, widely twisting in thin-walled structures, a scenario involving the application of dwell time is devised to mitigate associated issues. In the second approach, the MOOSE platform is employed to model the fully coupled thermo-mechanical phase field formulation, providing insights into the interrelated multi-physics and multi-scale phenomena in Selective Laser Melting (SLM) processes. This approach utilizes massively parallel finite element computations, treating powder particles as a homogenized continuum medium and accounting for heat transfer through conduction. The model aims to capture the nonlinear, non-equilibrium characteristics of the melt pool and various multi-physics phenomena in Powder Bed Fusion (PBF) processes, including powder layer generation, melting-solidification, phase changes, induced distortion, and residual stresses.

Additionally, a computational script is developed to predict secondary phases that emerge during cyclic loading with heating and cooling. This script employs the non-isothermal diffusion concept based on modified JMA model to calculate the phase fractions and couples it with the effect of the changing the temperature. To accurately capture phase transitions and their evolution, a phase field modeling framework is incorporated alongside the mean field computational stage. This integrated approach provides a comprehensive understanding of phase behavior under cyclic loading conditions. Furthermore, a novel closed-loop controller based on reinforcement learning is introduced to observe and control the evolution of the melt pool in terms of size and temperature. This approach holds great promise for real-world training of controllers, enhancing the capabilities of AM machines, and optimizing process parameters to achieve improved part quality and performance.

Keywords: Additive manufacturing, Finite element method, Phase Field, Multi-physics, Multiscale, Residual stress, Phase fraction, Inconel 625, ABAQUS, MATLAB, MOOSE, Reinforcement Learning

Resumo

Este estudo abrange diversos aspectos computacionais da modelagem de processos na manufatura aditiva (AM), com um foco particular na modelagem dissipativa de campo de fase para prever respostas térmicas, mecânicas e microestruturais. O crescente interesse na AM advém de suas possibilidades avançadas de fabrico; no entanto, uma compreensão abrangente da formação de defeitos e das respostas constitutivas/estruturais ainda é difícil de ser alcançada devido à natureza complexa multi-física do processo. Para enfrentar esses desafios, é necessária uma abordagem computacional confiável que considere os aspectos multi-escala e multi-física da AM. Técnicas numéricas avançadas surgiram recentemente, permitindo a previsão de defeitos com base em parâmetros do processo e facilitando a determinação de janelas de processamento ótimas para propriedades mecânicas desejadas. As simulações numéricas têm se mostrado ferramentas robustas, económicas e confiáveis para prever a qualidade de componentes na manufatura aditiva. Nesse contexto, este estudo tem como objetivo propor um modelo do processo que integre conhecimentos de engenharia computacional de materiais em processos de manufatura aditiva. O estudo utiliza duas abordagens: A primeira abordagem agrupa um modelo de campo de fase, termodinamicamente consistente, com um modelo de transferência de calor em regime transitório para rastrear as fases de estado do material. Essa abordagem divide o domínio em regiões correspondentes a diferentes estados separadas por uma interface difusiva. A variável de campo de fase, obtida a partir de soluções explícitas da Formulação de campo de fase de Wang, captura com precisão o grau de consolidação entre as fases de pó e fundida. Um modelo baseado em entalpia é incorporado para lidar com a não linearidade resultante do acoplamento das duas abordagens. A viabilidade de estudar a importância do banho de fusão é demonstrada por meio de simulações pelo método dos elementos finitos ao nível de processamento de uma camada de material usando o código comercial ABAQUS. As simulações são então estendidas para múltiplas camadas, permitindo a modelação de geometrias complexas e padrões de tamanho real. Ao considerar as propriedades do material dependentes do campo de fase e aproveitar as respostas térmicas, a equação de desigualdade dissipativa de energia permite a previsão de tensões residuais e deformações. Para explorar a influência dos padrões de escaneamento a laser em deformações estruturais, amplamente retorcidas em estruturas de paredes finas, é projetado um cenário envolvendo a aplicação de tempo de espera para mitigar problemas associados. Na segunda abordagem, a plataforma MOOSE é utilizada para modelar a formulação de campo de fase termomecânica totalmente acoplada, fornecendo informações sobre os fenómenos multi-físicos e multi-escala interrelacionados nos processos de “fusão seletiva por laser” (SLM). Essa abordagem utiliza cálculos de elementos finitos recorrendo a computação massivamente paralelizada tratando as partículas de pó como um meio contínuo homogeneizado e levando em consideração a transferência de calor por condução. O modelo tem como objetivo capturar as características não lineares e não equilibradas do banho de fusão e vários fenómenos multi-físicos nos processos de

“fusão em leito de pó” (PBF), incluindo a geração de camadas de pó, fusão-solidificação, mudanças de fase, distorção induzida e tensões residuais. Além disso, uma estratégia computacional é desenvolvida para prever fases secundárias que surgem durante o carregamento cíclico devido ao aquecimento e resfriamento. Esse código utiliza o conceito de difusão para calcular frações de fase hierárquicas e as combina com a temperatura. Para capturar com precisão as transições de fase e sua evolução, uma estratégia computacional de modelagem de campo de fase é incorporado juntamente com a etapa computacional de campo médio. Essa abordagem integrada proporciona uma compreensão abrangente do comportamento de fase sob condições de carregamento cíclico. Além disso, é introduzido um novo controlador de malha fechada baseado em aprendizado por reforço para observar e controlar a evolução da poça de fusão em termos de tamanho e temperatura. Essa abordagem tem grande potencial para o treinamento real de controladores, aprimorando as capacidades das máquinas de AM e otimizando parâmetros de processo para obter uma melhor qualidade e desempenho das peças.

Palavras chaves: Manufatura aditiva, Método dos elementos finitos, Campo de fase, Multi-físicas, Multi-escala, Tensão residual, Fração de fase, Inconel 625, ABAQUS, MATLAB, MOOSE, Aprendizagem por Reforço.

Chapter 1

Introduction

1.1.Introduction

In recent decades, additive manufacturing (AM) processes have garnered significant attention and enthusiasm within the manufacturing sector. This burgeoning technology, particularly in the context of Inconel 625 and metal additive manufacturing, has witnessed a meteoric rise in popularity over the past two decades [1]. Originally conceived as a means for rapid prototyping of metallic components, AM processes have evolved into a groundbreaking method for translating virtual three-dimensional (3D) computer-aided designs into tangible reality. The key principle underlying AM is the layer-by-layer deposition of material particles onto a substrate plate, orchestrated by a high-intensity heat source, which can be a laser or an electron beam [1][2]. This innovative approach, owing to its unparalleled capability to create structurally-sound, intricately designed components, has found extensive acceptance across a spectrum of industries, encompassing bioengineering, aerospace, medical, defense, and automotive sectors [2]. AM offers a multitude of advantages over traditional manufacturing methodologies, including the capacity to fabricate complex geometries with superior strength, thermal properties, and wear resistance. It is also environmentally friendly, as it significantly reduces material wastage and eliminates the need for additional tools and dies due to its virtual-to-reality transition from computer-aided design (CAD) to computer-aided manufacturing (CAM) [3][4]. In the realm of AM, two prominent categories of techniques have gained prominence: powder bed systems and powder-wire fed systems. Both categories rely heavily on the synergistic integration of CAD and CAM, constituting highly efficient means of producing medium-to-large-sized components that closely approximate the desired near-net shape [3][4]. In the case of Inconel 625, a highly regarded material in these advanced processes, the challenges and opportunities are magnified, as this nickel-based superalloy is known for its exceptional corrosion resistance, high strength, and elevated temperature properties, making it a material of choice in aerospace, marine, and chemical processing industries. However, its processing in AM poses unique challenges, and the need for precise control and understanding of its behavior during additive manufacturing is paramount. Unlike the conventional powder bed fusion (PBF) approach, which spreads a layer of powder over a bed and selectively melts it with a heat source, directed energy deposition (DED) AM systems employ a nozzle mounted on a multi-axis arm heat source. In DED, material is deposited on a substrate plate through the melting and solidification of a feedstock material, which can be in the form of wire or powder. This differentiation in AM techniques underscores the versatility of the technology and the diverse array of materials it can accommodate, including the demanding Inconel 625 [3]. Despite the immense promise of metal additive manufacturing, when juxtaposed with conventional manufacturing techniques, several potential forms of defects loom on the horizon that can compromise the overall quality of the final Inconel 625 components [5]. These defects are a direct consequence of the inherent complexity of the AM process [6]. Typically, resolving such issues necessitates an empirical, trial-and-error approach, involving experimental

tests to ascertain the optimal process parameters for achieving the desired quality. This experimental methodology encompasses a wide spectrum of techniques, ranging from light optical microscopy (LOM) and scanning electron microscopy (SEM) to observe meso-scale defects such as porosities and grain shapes [7,8]. Additionally, techniques like Electron Back-Scattered Diffraction (EBSD) and X-ray Computed Tomography (X-CT) come into play for visualizing grains and identifying porosities within the Inconel 625 samples [9]. These experiments, termed ex-situ methods, primarily transpire after the AM process's completion and provide extensive information on both micro and macro scales. However, they fall short in elucidating the underlying mechanisms governing defect formation and initiation.

- **In-Situ Monitoring and Numerical Simulation:**

Concurrently, the field has seen a rise in in-situ monitoring techniques such as infrared thermal imaging and X-ray monitoring [10], offering more detailed insights into the evolution and genesis of defects throughout the manufacturing of Inconel 625 parts. Nevertheless, it is essential to acknowledge that in-situ monitoring approaches demand meticulous preparation and precise calibration. As an alternative, numerical simulation emerges as a cost-effective avenue to complement or even supplant in-situ monitoring [10]. A pivotal attribute of numerical simulation is its inherent flexibility, as it can be readily modified and adapted based on empirical assessments. This flexibility enables the modeling and analysis of complex physical processes that are otherwise challenging to monitor directly. The trajectory of numerical simulation in the context of AM can be traced back to the 1970s when authors like Hughes [11] and Zeinkiewicz, Taylor, and Zhu [12] pioneered the solution of heat transfer problems through finite elements. In the early 1990s, finite element methods (FEM) began to be employed in the simulation of selective laser sintering (SLS) [13]. Over the subsequent decades, various endeavors have been undertaken to model the thermomechanical processes involved in DED AM using FEM, employing a diverse range of commercial software or in-house codes [14–20]. In 2017, Meier et al. [21] introduced a comprehensive classification of heat modeling specific to selective laser melting (SLM), focusing on different length scales. This classification allowed for the incorporation of physics at various length scales, enabling the exploration of phenomena such as dendrite growth [22], melt pool studies at micro [23] and meso [24] scales, as well as investigations into stress formation [25] [26] and crack propagation [27] at both micro and macro scales. The complexity inherent to the AM process stems from two primary sources: (i) the multi-physics nature of the process, encompassing intricate interactions with various physical phenomena, and (ii) multiscale characterization, indicating that different phenomena can occur at specific length scales [28]. Moreover, the modeling endeavor is further compounded by the fact that certain physical processes transpire within an extremely short timeframe, often on the order of microseconds. In the realm of AM, an ephemeral interaction unfolds between the powder

particles and the high-energy laser beam before the powder particles enter the melt pool. This interaction induces laser energy attenuation [28] and a non-linear temperature increase in the powder particles [29]. Properly accounting for this interaction, the consolidation of the powder, and the solid-liquid phase change is essential in the numerical model [30][31]. In any arbitrary computational domain near the laser source, three distinct material phases are encountered: powder, molten, and solidified. These phases exhibit significantly different mass densities, resulting in phase changes that elicit relevant process-induced eigenstrains [30][31]. Addressing these nuances entails considering different approaches to model phase changes, such as enhancing the Stefan-Neumann equation [32] or employing specific phase change functions [33]. In another effort a thermodynamically phase field model for solidification proved to be useful to capture the consolidation of the material, allowing to investigate the phase-dependent laser absorptivity [34]. Some models treat the powder as a continuum and simulate local melting in the vicinity of the laser, typically in a single layer or a few layers [35][36]. On a larger scale, 3D thermal-mechanical finite element models have been instrumental in predicting residual stresses and distortion in plates [37] and warping during the construction of simple parts [38]. Despite substantial efforts to develop reliable models for predicting temperature fields, melting stages, re-solidification, residual stresses, and distortion during material deposition in metal additive manufacturing [39][40][41], a knowledge gap persists, particularly concerning the refinement of process-structure-properties relationships. The enigma of unexpected material behavior can be attributed to non-uniform rapid thermal fluctuations during the laser heating and cooling cycles intrinsic to layer-wise AM processes. This phenomenon induces complex microstructural evolutions, particularly in multiphase alloy systems like Inconel 625 [42][43]. To explore these microstructural intricacies at the mesoscale, well-established models, including Monte-Carlo [44] and phase-field [45,46] methods, have been coupled with thermal simulations to discern the melt pool's grain structure evolution.

- **Integration of Mean field and Phase Field Modeling:**

In the context of mean-field and phase-field modeling, the phase field method [47–49] stands out as a powerful simulation framework that excels in predicting transformation diagrams and the evolution of precipitate morphologies during metal additive manufacturing (AM). This approach uniquely considers local non-equilibrium conditions arising from the rapid heating and cooling cycles inherent to the AM process. While the phase field method provides valuable insights into microstructural evolution, there is significant untapped potential for further developments in process control to enhance AM techniques, improve material properties, and reduce variability in inter-build outcomes and the occurrence of embedded material discontinuities. Concurrently, Avrami [50] introduced a diffusive model that relates the evolution of microstructures to time and temperature. This model proposed a two-stage transformation mechanism involving the

nucleation of new phases followed by their growth in volume, with the rates of these stages governed by a temperature function. Leveraging this methodology, a computational framework emerges, utilizing the thermal field generated during the AM process to predict thermal maps, localized temperature gradients, and cooling rates. This framework integrates microstructure data from previous steps through a structure-property link, typically employing mean-field-based methods that provide valuable information, including time-temperature-transformation (TTT) and continuous-cooling-transformation (CCT) diagrams, which are applicable to a wide range of systems. However, it's worth noting that while these methods can successfully predict the fraction of phase evolution, forecasting the morphological evolution remains a challenging task. Consequently, the phase-field modeling (PFM) framework proposed in this study holds immense promise for application to multi-phase alloys, with several distinct advantages over other models such as Svoboda-Fischer-Fratzl-Kozeschnik (SFFK) [51] and Lifshitz-Slyozov-Encounter-Modified (LSEM) [52]. Firstly, the phase-field model leverages lattice misfit strain between precipitated phases and the matrix as input, enabling it to accurately predict the evolution of the phase's aspect ratio without the need for extensive calibration against experimental data. Secondly, the phase-field model has the unique capability to capture particle growth under elastic stresses and compositional strains, making it a natural choice for simulating the "directional encounter" phenomenon observed in precipitations.

- **AI and Closed-Loop Control:**

Process control in the realm of in-situ monitoring and the enhancement of material properties, coupled with the goal of reducing inter-build variation and minimizing embedded material discontinuities, necessitates the development of robust process monitoring methods. These methods serve as precursors to the production of high-quality, defect-free products, thereby rendering the additive manufacturing (AM) process more sustainable. Notably, significant research efforts have been dedicated to modeling the time-varying melt pool in AM, broadly falling into two categories: (i) characterizing the melt pool based on morphological characteristics and (ii) capturing the thermal characteristics of the melt pool. The first group of studies [53,54] is focused on capturing changes in the size, length, depth, area, and other geometric features of melt pools during the fabrication process, often utilizing cameras and sensors for data collection. In contrast, the second group concentrates on empirical temperature measurements over the melt pool, including parameters like peak temperature and average temperature [55,56]. Classical optimization methods have historically been employed to devise control strategies aimed at reducing the occurrence of mechanical defects during AM. However, these methods are constrained by the need for severe model order reductions and are limited in their ability to process extensive data due to computational constraints [56][57]. In alignment with these research trends, recent years have witnessed a growing interest among researchers in the application of Artificial

Intelligence (AI) in various domains related to metallic additive manufacturing (MAM). This interest encompasses areas ranging from the prediction of material properties to the control of the manufacturing process itself. Given the pivotal role of melt pool characteristics in assessing the quality of AM-produced components, the present study delves into process monitoring and laser power control to shed light on the influence of process parameters on instabilities occurring at the scale of the melt pool. From our perspective, there has yet to be an existing integrated framework that comprehensively considers both the mechanical material model and phase change phenomena in a physically well-motivated manner. This gap presents a compelling opportunity to explore the integration of AI and closed-loop control systems into the AM process, with the aim of optimizing and enhancing the production of high-quality components while mitigating defects and irregularities.

1.2. Research objectives

The overarching objective of this research is to advance the understanding and control of metal additive manufacturing (AM) processes, with a specific focus on the in-situ monitoring and enhancement of material properties. This objective is pursued through the development and implementation of novel phase field modeling frameworks and the integration of AI-driven closed-loop control systems. The research is organized into two distinct but interconnected endeavors:

- **Multi-Physics Phase Field Modeling for AM Processes:**

Develop a comprehensive computational framework for additive manufacturing (AM) that integrates dissipative phase field modeling to predict thermal, mechanical, and microstructural responses. This framework aims to address the complex multi-physics nature of AM, allowing for a deeper understanding of defect formation and constitutive/structural responses.

- **Integration of Integrated Computational Materials Engineering (ICME) in AM:**

Propose a process model framework that incorporates insights from integrated computational materials engineering (ICME) into AM processes. This approach seeks to utilize advanced numerical techniques to predict defects based on process parameters and determine optimal processing windows for desired mechanical properties.

- **Two Approaches to Phase Field Modeling for Process Modelling:**

Develop and validate two distinct classes of phase field (PF) models within the computational framework. The first approach couples a thermodynamically consistent phase field model with a transient heat transfer model to track material phase states, allowing for the study of melt pool behavior and energy dissipative inequality. The second approach employs the MOOSE platform

to model fully coupled thermo-mechanical phase field formulation for Selective Laser Melting (SLM) processes, focusing on the interrelated multi-physics and multi-scale phenomena.

- **Prediction of Phase Fraction Evolution Under Cyclic Loading:**

Develop a computational script to predict secondary phases fraction that emerge during cyclic loading with heating and cooling for Inconel 625 super alloy. This script incorporates non-isothermal diffusion concepts and integrates a mean field modeling framework to provide a comprehensive understanding of phase behavior under these conditions.

- **Closed-Loop Controller Integration:**

Integrate a novel closed-loop controller based on reinforcement learning with the simulation environment to observe and control the evolution of the melt pool in terms of size and temperature. This controller holds the potential for real-world applications in enhancing AM capabilities and optimizing process parameters for improved part quality and performance.

1.3. Research motivation

While additive manufacturing (AM) holds immense potential, it is not exempt from its share of challenges. The intricate interplay of physical phenomena within AM processes presents formidable obstacles in achieving consistent part quality, minimizing defects, and optimizing material properties. In response to these challenges, researchers and engineers have turned to computational methods to gain profound insights into the intricate nature of AM. These computational tools are instrumental in developing strategies aimed at enhancing the reliability and efficiency of the process. In this context, our research endeavors are dedicated to addressing critical aspects of AM by harnessing the capabilities of advanced numerical simulations and phase field modeling. Our primary objectives include devising solutions for monitoring, controlling, and optimizing AM processes. Ultimately, our goal is to contribute to the production of high-quality components with significantly reduced defects. To provide insight into the motivations driving our research, we present a comprehensive list below:

- **Complexity of AM Processes:**

Additive manufacturing (AM) processes offer advanced manufacturing possibilities, but their complex multi-physics nature presents challenges in understanding defect formation and material responses. Reliable computational approaches are needed to address these challenges comprehensively.

- **Role of Numerical Simulations:**

Numerical simulations have proven to be robust, cost-effective, and reliable tools for predicting component quality in AM. They provide an alternative to time-consuming and costly experimental methods, enabling the study of complex AM processes.

- **Integration of ICME:**

Integrating insights from integrated computational materials engineering (ICME) into AM processes can enhance the control and predictability of AM processes. This integration allows for the development of optimized processing parameters and defect prediction.

- **Phase Field Modeling:**

Phase field modeling offers a versatile approach to studying phase transitions and microstructural evolution during AM. The proposed phase field models aim to capture the behavior of melt pools, energy dissipation, and phase consolidation accurately.

- **Cyclic Loading and Phase Evolution:**

Understanding phase behavior under cyclic loading conditions is crucial for predicting material responses accurately. The integration of non-isothermal diffusion concepts and phase field modeling provides insights into phase evolution during cyclic loading.

- **Closed-Loop Control:**

Integrating a closed-loop controller based on reinforcement learning holds promise for real-time control of AM processes. This controller can optimize process parameters and improve part quality, making it a valuable tool for AM applications.

1.4. Thesis organization

This thesis is organized into eight chapters as follows:

Chapter 1 focuses on the introduction, research objectives and motivations.

Chapter 2 provides a brief overview of two metal additive manufacturing technology including direct energy deposition and selective laser melting, its pros and cons, limitations, and possibilities.

Chapter 3 presents typical numerical methods for AM process modeling, including dynamic approaches and methods for tracking irregular boundary conditions. It also provides an overview of phase change phenomena modeling.

Chapter 4 explains the theoretical formulation for AM processes in detail, covering two different approaches: the uncoupled and fully coupled PF models. It demonstrates how coupling the phase field approach can govern the irreversibility of phase changes for powder and track the solidification frontier. Additionally, the incorporation of Helmholtz free energy to satisfy the

second law of thermodynamics is discussed for calculating residual stress and inducing distortion. The chapter also describes the development of a computational code to predict secondary phases accurately during cyclic loading, using the concept of non-isothermal diffusion and phase field modeling.

In **Chapter 5**, the numerical simulation procedure for additive manufacturing is implemented using the ABAQUS platform for the DED process. Additionally, modeling of SLM processes is performed in conjunction with the MOOSE platform. The implementation of finite element methods regarding governing residuals in weak forms is also presented for the proposed PF models.

Chapter 6 describes and assesses numerical results in comparison with experimental results.

Chapter 7 introduces a closed-loop controller to observe numerical simulations at a melt pool scale using reinforcement learning (RL) solutions.

Chapter 8 outlines conclusions and suggests future study directions.

Chapter 2

Additive Manufacturing (AM) Technology

2.1. Introduction

Additive manufacturing (AM), also known as 3D printing, is the general term for those technologies that create digitally 3D physical objects by successive addition of material. In additive manufacturing, a 3D object is usually built from a digital model into its designed shape using layer by layer process. In comparison with formative (eg. casting, forging, mold or dies, plastic injection) or subtractive (e.g. carving, milling, drilling, grinding) manufacturing, additive manufacturing is fundamentally different in methodologies and it can significantly simplify the process of producing complex 3D objects. Nowadays, Additive manufacturing technologies have already been used for various applications in the engineering industry as well as other areas of society, such as medicine, education, architecture, entertainment, jewellery, and so on [6]. All AM machines presently use a layer-based approach, in which each layer is a thin cross section of the part derived from the original Computer Aided Design (CAD) data [58]. The final part made by AM technology can be considered as a geometrical approximation of the originally designed data. The additive manufacturing is broadly applicable in different material categories, including metals, ceramics, polymers, composites and biological materials. Correspondingly, additive manufacturing applies different technologies for the material joining process. Hence, the categories of additive manufacturing technologies are still increasing with the rapid development of AM in both industrial and academic research.

2.2. Advantages

Additive manufacturing provides many opportunities to design and improve products. Since the first stereolithography fabrication system in the 1980s, additive manufacturing has been revolutionizing the way things are made for more than 30 years. The product portfolio and product life-cycle, such as design (CAD), engineering (CAE), manufacturing (CAM), and manufacturing operations management (MOM), will benefit from the advantages of AM technologies (see Figure 1), including:

- (i) Geometrical complexity: weight is an important parameter in the automotive industry and aeronautic industry, correlating to fuel consumption; additive manufacturing's flexibility in highly complex geometries gives the designer more freedom during the design process to optimize the product; the lightweight design of parts can be developed with fewer manufacturing constraints after topology optimization.
- (ii) Less assembly: in additive manufacturing, combining features into single-piece parts greatly reduces detailing screw holes and assembly drawing [59]; therefore, AM technology is an alternative option for solving geometric dimensioning and tolerance (GD&T) issues in assembly.

- (iii) Less waste of material: in comparison with subtractive manufacturing, the required material can significantly reduce in additive manufacturing; it can minimize the use of material while the part's strength/weight ratio is still retained after optimization.
- (iv) Highly customizable on-demand production: with AM's help, manufacturers can increase the diversity of product offerings that are currently too small to specialize due to mold, die, or tooling costs; with a more affordable price, the consumer can buy built-to-order products more closely suitable for individual needs and wants; without the need for molds and dies, AM enables the engineers or designer to try multiple iterations simultaneously with less cost.

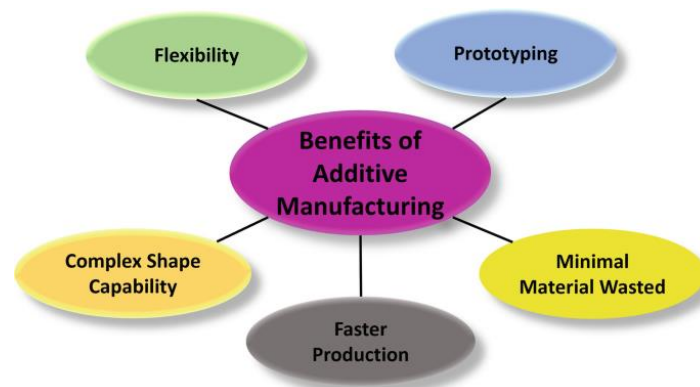


Figure 1 schematic of AM advantage [60].

2.3.Limitations

Additive manufacturing has distinct advantages and disadvantages. Thus, AM is not always the best choice for all products. Before the application of additive manufacturing, designers and engineers should consider the trade-off between its benefits and limitations. Some limitations restrict the application of AM technology, and overcoming these problems is still challenging for scientists and researchers. These limitations are partially summarized as follows:

- (i) Poor mechanical properties and excessive distortion: due to the layer-by-layer fabrication process, some properties of a part are usually not isotropic; therefore, parts made by some AM technologies, especially metallic parts, are often weaker in strength and endurance than their traditional manufacturing counterparts; distortion may occur in the AM process, leading to an inferior shape quality and even to the ceasing of the fabricating process.
- (ii) Hardware expense: compared to conventional manufacturing machines, additive manufacturing is relatively more expensive for large production runs; specialized equipment, such as devices of high-voltage power supply, is essential for some AM

machines; some auxiliary modules should be installed as well; for example, large numbers of ultra-fine powder or some hazardous volatile organic compounds may be emitted during printing; devices treating harmful emissions are indispensable in these AM systems; the integration of sophisticated devices makes the price of AM machines still expensive for industrial applications.

- (iii) Limited component size and slow build rate: many AM machines lay down material in small building chambers, and it assures printing resolution with nozzles or other delicate deposition devices; the AM system's limited volume and material deposition speed often make additive manufacturing less competitive in part size and building rate than conventional manufacturing.
- (iv) Difficult process configuration and control: AM machine works digitally from CAD files to its final part; it involves many process parameters impacting the final quality of the product; the configuration and control are usually empirical on AM machines; If one factor is changed in AM, the other parameter should be re-determined after a series of trials; this is why some AM machine companies often sell their machine bundled with their unique raw material; configuring and controlling these parameters during the process relies on a better understanding of AM systems and hardware improvement.

2.4. Typical metal additive manufacturing technologies

Different AM technologies can be distinguished by the material chemical composition, including paper, polymers, wax, resins, metals, ceramics, and their mixture [64]. Extensive knowledge of the material is necessary for an appropriate choice of forming methods. Metal is one of the essential materials widely used in current AM systems. Metals generally have higher yield strength than other conventional structural materials. Their applications for AM systems are widely researched because of their important role in the industry, architecture, jewellery, bio-medicine, etc. Nevertheless, for some metal AM systems based on melting or sintering, heat processes such as sintering during manufacturing will cause rapid temperature gradients, and residual stress or cracking occurs. Nowadays, metal AM technologies still have some severe problems in comparison to conventional subtractive metal manufacturing. Laser and electron beams are usually used as heat sources in metal AM systems. A final workpiece fabricated by additive manufacturing is usually a solidified object. However, the joining process depends on the different initial states of raw materials in different AM systems [61]. Powder materials are usually used for metal printing. Powder material can be processed by partially or fully melting and fusing together, creating a solid part with "powder bed fusion" or "directed energy deposition" technologies. A laser or electron beam can be used to melt the powder. Also, the powder can be glued by a special substance called a binder. The physical properties of discrete metal powder and

a solidified metal sample are generally different because of their scale differences. In the development of AM technologies, patents significantly influence the technical solution. During the validity of one patent, relevant companies often work on similar basic AM systems with particular specific improvements, which makes the terminology of AM technologies quite ambiguous and confusing. Different companies often name their AM system with different names to apply for patents, even though the fundamentals of their approaches often have similarities. Here we will review commercialized AM technologies neglecting details of differences between AM companies and trademarks. Different metal additive manufacturing technologies are introduced in the following.

2.4.1. Powder-based additive manufacturing

This thesis mainly concentrates on the AM technologies dedicated to fabricating metallic parts. Currently, most of the popular metal AM systems in the industry are based on powder bed or powder injection.

2.4.1.1. Powder-bed based technologies

Selective Laser Sintering (SLS) and Selective Laser Melting (SLM) are two kinds of powder-based AM technology [62]. The equipment of SLM and SLS are similar. At the same time, the usual materials used in these two systems are different: SLM generally works with metal, such as stainless steel, aluminum, and titanium alloys, as shown in Figure 2. SLS (Figure 3.) usually works with plastics, glass, ceramics, etc. In these systems, a thin layer of heat-fusible powder is deposited onto the part-building chamber. Laser devices and optics scanning mirrors are installed above the powder bed in the vacuum or inert-gas-filled chamber. The powder is held in a cartridge which may be pre-heated by infrared. The build platform moves downwards by one layer of thickness after one layer of a part is built. Then the new powder layer will be spread uniformly and precisely onto the previous powder bed by a leveling roller or a blade. After the deposition of the new powder layer, the zone of the cross-section of layers is melted or sintered selectively by the heat of the laser. In SLS/SLM system, the support of part is not necessary since the powder bed can support a newly built cross-section layer. The post-process is quite important for these technologies as the whole part must be cooled down slowly to avoid warping and curling.

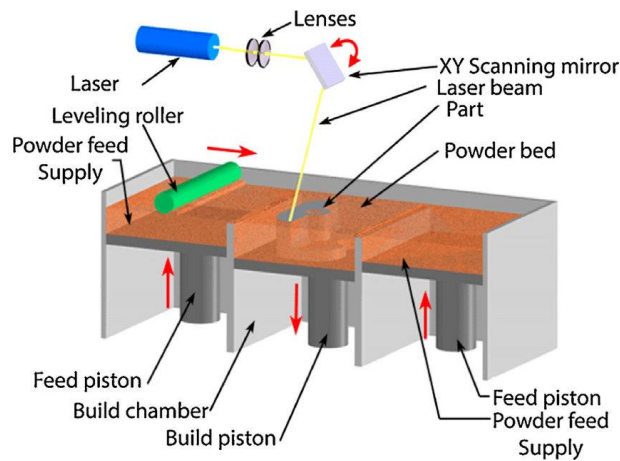


Figure 2 Selective laser sintering\melting.

In SLM, the powder is melted, and the material consolidates in a welding pool; a schematic picture is shown in Figure 4. This different feature makes the final part made by SLM have less porosity than that produced by SLS, as the powder is heated below its melting point in SLS (see Figure 4). In SLS, a solid is formed by the fusion between material particles (sintering). For both systems of SLM and SLS, the control of laser energy input is significant for the quality of the part [63]. The parts made by SLM/SLS often require stress relieving and annealing to reduce internal residual stress.

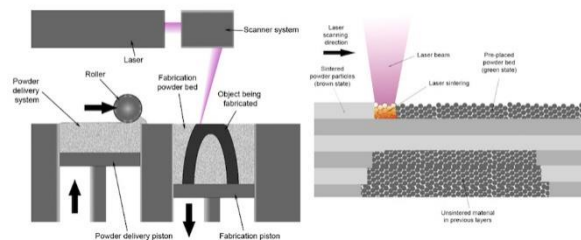


Figure 3 Interaction of laser material in selective laser melting (SLM).

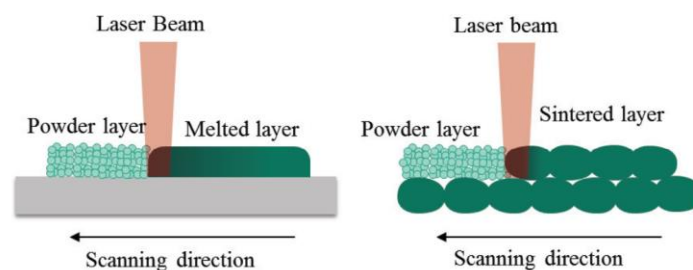


Figure 4 Difference of SLS and SLM [63].

Electron beam melting (EBM) is an AM technology similar to SLS/SLM [64]. The EBM (Figure 5) uses an electron beam as a heat source instead of a laser, as in SLS/SLM. Only materials with high electrical conductivity can be used in EBM technology. In the EBM system, the electron beam is focused by a deflection coil surrounding the beam. The movement of electron beams focus is driven magnetically instead of the mirror galvanometers in SLS/SLM. Because of the different mechanisms between the interaction of material/electron beam and that of material/laser, EBM is much more efficient in energy absorptivity.

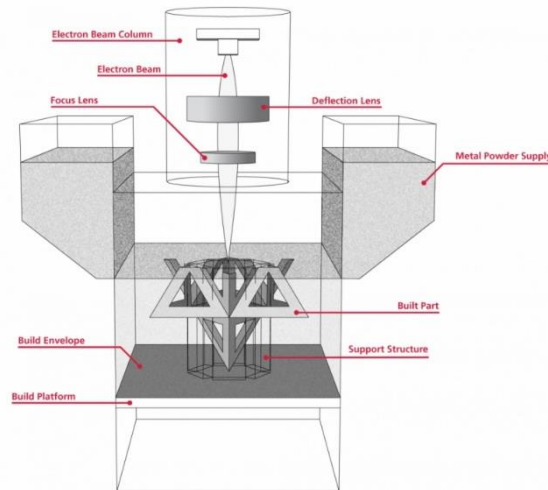


Figure 5 Electron beam melting (EBM).

Compared to SLS/SLM systems, parts made by EBM technology generally have less precision, worse surface resolution, and bigger grain sizes. However, EBM has advantages in less cost and faster scan speed. This makes EBM an important technology in metal additive manufacturing.

2.4.1.2. Powder-injection based technologies

Direct Energy Deposition (DED) is a typical powder-jet-based AM technology [65]. This technology can be used to manufacture new parts, repair/rebuild worn or damaged components, and apply wear- and corrosion-resistant coatings [66]. In the DED system, the metal powder is injected from the coaxial nozzle (see Figure 6) into a molten pool, which is created by a heat source (usually a laser). The powder nozzle moves with the laser beam back and forth, then leaves a track of solidified material. Shield inert gas is also fed with the sprayed metal powder stream. The DED printer head (nozzles of powder/inert gas, laser beam) is usually integrated into CNC/robotic system. With some feedback sensors for melt pool, DED can be controlled by a closed loop to maintain the quality of a part.

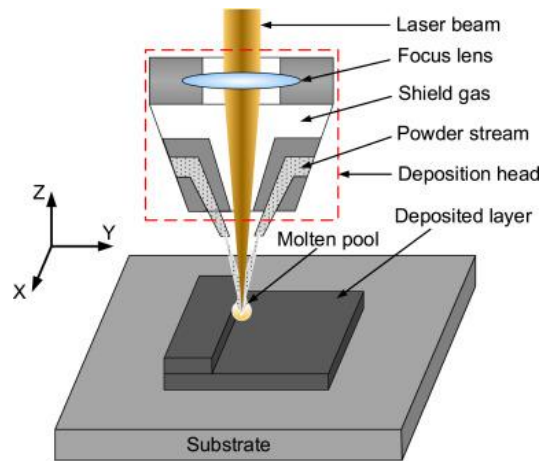


Figure 6 Laser energy deposition (DED).

The DED involves complicated interactions between the laser beam, metal powders, the substrate, and processing gases. The physical phenomena in DED include laser powder-melt pool interactions, heat transfer, fusion, fluid flow, and solidification. Compared with powder bed-based AM technologies, the printing speed of DED is faster with higher roughness, and DED allows for building or repairing larger parts. DED technology isn't only applied in the additive manufacturing of new parts but also in the refurbishing-repairing of damaged parts. Laser Engineered Net Shaping (LENS) and laser cladding are powder-injection-based AM technology similar to DED technology [67] because they are different patents issued to companies or individuals.

2.5. List of challenges in metal additive manufacturing

In the industrial sector, in the application of metal additive manufacturing, the quality of a metallic part may not be satisfactory in terms of geometrical shape and properties. Some severe problems on the macro-scale may even lead to the cease of fabrication. Here are some typical macroscopic problems in metal additive manufacturing. Solutions for these issues are still being studied by researchers with experiments or simulations.

2.5.1. Considerations before the AM process

Before the printing process of additive manufacturing, engineers or scholars need to consider some induced problems, including: (i) Material selection: Choosing the suitable material for the intended use can be challenging, especially as a wide variety of materials are available for different additive manufacturing processes. (ii) Design optimization: Designing parts for additive manufacturing requires a different approach than traditional manufacturing methods. It can be challenging to optimize designs for printing without sacrificing strength or other functional requirements. (iii) Software compatibility: Different 3D printing software may have different file

formats or requirements, making it challenging to ensure that the design files are compatible with the printing process.

2.5.2. Problems during the AM process

In the printing stage, it is mandatory to monitor the property and shape of the parts since AM parts quality is not always satisfactory breed from

- (i) Printing accuracy: maintaining accurate print dimensions and avoiding errors in the printing process is essential for producing functional parts.
- (ii) Build quality: ensuring consistent layer adhesion, avoiding warping or delamination, and controlling the temperature and humidity during printing can all impact the quality of the final part.
- (iii) Process monitoring: monitoring the printing process in real-time to detect errors or deviations from the expected output can be challenging, especially for long prints.

2.5.3. Problems after printing of an AM part

Most challenges after finishing the AM process arise from:

- (i) post-processing: removing support structures, smoothing surfaces, and applying finishing treatments can be time-consuming and require specialized equipment and expertise.
- (ii) Quality control: ensuring the final part meets the desired specifications can be challenging, especially for complex geometries or parts with critical tolerances.
- (iii) Recycling and waste management: managing the waste generated during printing and post-processing and finding sustainable ways to recycle or dispose of it can be challenging.

Chapter 3

Introduction to some typical numerical techniques for AM simulation

3.1.Introduction

Regarding the extensive and expensive experimental considerations required to measure the evolution of multi-physics involved fields in the additive manufacturing process, there is always a hardware limitation when it comes to simulation. Numerical simulations, especially macroscopic simulations for the AM process, provide an essential alternative for engineers and researchers. Due to the complexity of the AM process, these simulations often utilize specific methods to solve the multiscale and multi-physics problems involved. In this context, a brief introduction to the tendencies of AM simulations is presented.

3.2. Numerical methods for dynamic AM process

Concerning the dynamic nature of AM processes, from aspects of deposition of a material layer on the top of the substrate or its previous layers, all complex phenomena present (stacking of material, moving heat source, the interaction of new melt powder/solidified metal, etc.) require some particular numerical method.

3.2.1. The “element birth and death technique” in FEM

The "element birth and death technique" is broadly used in finite element method (FEM) frameworks like ANSYS, ABAQUS, COMSOL, etc. For a system simulation, the "element birth and death technique" can deactivate or reactivate selected elements wherever the material is added or removed. Most AM simulations based on FEM, including academic research or industrial design, have applied the "element birth and death technique" to treat the geometrical deformation process in additive manufacturing. This method can be helpful in modeling some effects due to phase changes (as in welding processes, when structurally inactive molten material solidifies and becomes structurally active), failure-surface propagation, and other analysis-dependent element changes. The drawback of this method can be referred to the identification of the elements prior to activation or deactivation procedures, which means the change of material status in these elements (for example, melting, solidification, rupture, etc.). In the "element death" step, the element does not actually is removed. In fact, the stiffness (or conductivity, or other analogous quantity) of these elements is multiplied by a severe reduction factor (in ANSYS, this factor is set to 1.0×10^{-6} as default [73]). Element loads associated with deactivated elements are zeroed but still appear in element-load lists. Similarly, mass, specific heat, damping, and other such effects are set to zero for deactivated elements. The energy and mass of deactivated elements are not included in the model. Whenever an element is "killed", the element's strain is also set to zero. The element "birth" step is manipulated in a reverse manner. When an element is reactivated, its mass, stiffness, element loads, and other values return to their full original values. In the reactivated elements, strain (or heat flux, etc.) history is not recorded, while the initial strain,

defined as a constant, will not be affected by this birth and death method. The element types are also reactivated in their originally specified geometric configuration. The activation of element type should be specially treated when large-deformation effects happen in order to obtain meaningful results. During the AM process, the stress-free option can be applied to simulate newborn elements and previously-deposited elements. Especially in powder-bed-based AM simulation, the influence of powder surrounding the workpiece can be treated by these possibilities.

3.2.2. Discrete element method

The Discrete Element Method (DEM) is a numerical approach used to simulate the behavior of both continuous and discontinuous material systems, as illustrated in Figure 7. DEM simulations are based on Newtonian interactions among a system of particles. These particles are equipped with constitutive behaviors, including contact/collision models, heat transfer models, and the ability to form and break inter-particle bonds while responding to external fields. For the simulation of powder-bed-based AM technologies or powder-injection-based technologies at the microscale, a comprehensive reference on DEM applications can be found in [74], particularly for simulating the melting pool. Moreover, the DEM method has been extended to simulate macro-scale AM processes like the recoater blade/roller deposition process. In AM simulations, powder particles are geometrically simplified as spheres. DEM is a numerical approximation method that involves an interacting system of particles. By tracking a sufficiently large number of particles, reliable statistical analysis of granular dynamics becomes feasible. Some particles are in contact with each other, while others remain unbounded. Unattached particles participate in collisions, producing reaction forces that propagate, altering the particles' velocity and position. In DEM, particles also conduct heat transfer, respond to external fields, and may form or break inter-particle bonds. Prior to using DEM, it is crucial to define inter-particle contact laws and boundary condition contact laws. For simulations involving consolidation or melting, conditions for bond formation, deformation, and breakage should also be defined. Due to the impracticality of exhaustively checking every particle for contact with all others, collision detection techniques are employed to reduce collision searching to local neighborhoods.

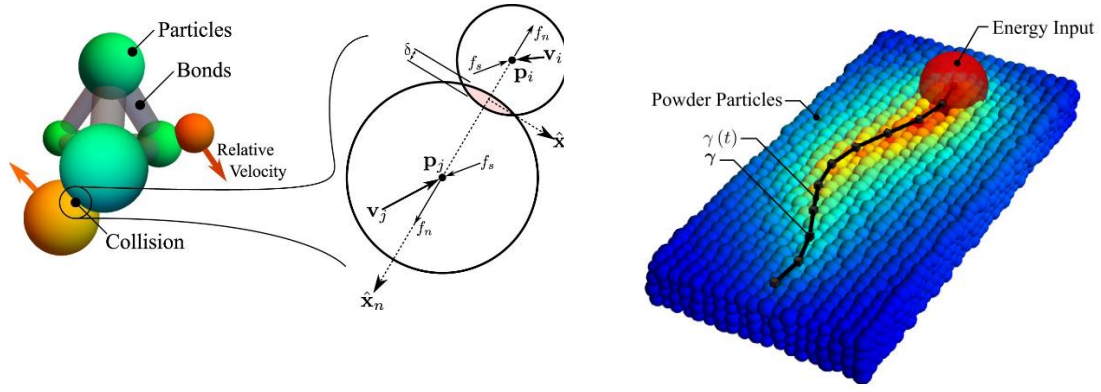


Figure 7 Overview of the Discrete Element Method. At right, the variables associated with the collision mechanics are depicted [68].

3.2.3. Mesh adaption

The mesh may act as a bottleneck with its critical role in the FEM concept, as the simulation time is proportional to the number of elements. AM simulations are executed for multi-scale models of the melt pool, hatch pass, layer, and the whole part, which makes the mesh adaptation a powerful tool to satisfy the different accuracy of details while trying to limit the simulation time. In the simulation of additive manufacturing, the mesh density needs to be adjusted spatially according to the mesh density needs and the need for detail required. Therefore, the whole mesh may be divided into two or three areas. Different mesh densities may be applied to the working, transition, and far-field areas. As shown in Figure 8, the geometry of the workpiece temporally evolves while the material is deposited. The mesh should also be dynamically adapted to adjust the local mesh refinement to the position of the laser spot or the current printed layer. In each analysis step, the dynamic mesh refinement (DMR) approach updates the mesh of the laser spot place after calculating the mesh metric matrix, which depends on the minimum curvature radius of the workpiece's free surface and the mesh node's distance from the interface.

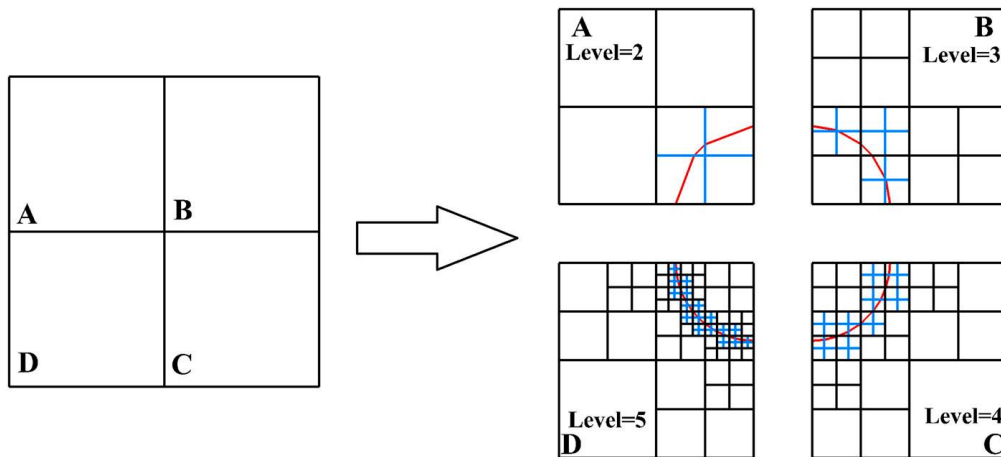


Figure 8 Illustration of block-structured grids with four different refinement levels: red contour for the frontier fluid interface; blue lines for the refined blocks; black lines for the bigger blocks.

3.3. Numerical solution for irregular and free boundary conditions

The process of AM depends on the geometry and shape of a 3D part. Considering the moving free surface is still very difficult for additive manufacturing simulation. Most investigations that precisely account for the free surfaces are in the microscopic and multiphase fluid dynamics category. Herein, the proposed strategies are sorted.

3.3.1. Voxelization of complex geometries

In 3D computer graphics, a voxel is a straightforward generalization of a pixel as known from computer concept. The space is split into a regular cubic grid consisting of voxels. The easiest way to represent an object with voxels is to assign to each voxel a Boolean value, deciding if the volume described by the voxel is part of the object or not [68]. In the voxel-based approach, voxels do not necessarily need to be cubes but can be cuboids with different side lengths, as shown in Figure 9. In AM simulations, voxels can be the same as the elements' concept in FEM. Nowadays, the problem of voxel-based representation is its huge memory consumption for high resolution. This problem still needs to be solved through some algorithms, such as octrees [69] that are used to reach a compromise between memory consumption and geometrical accuracy of representation. In voxel-based representation, the concept of feature edges or feature surfaces is no more necessary as boundary representation.

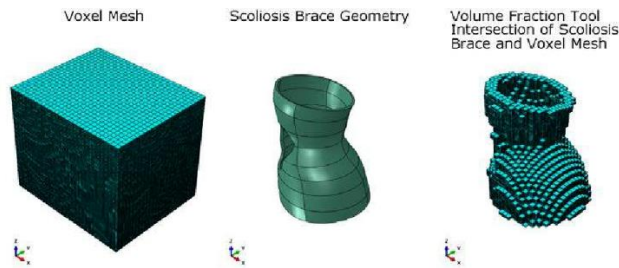


Figure 9 A scoliosis-brace-model reconstructed by voxelization [70].

3.3.2. Level set method

The level-set method (LSM), originally proposed by Osher and Sethian [71], is an implicit method to capture a moving front. This method relocates the interface position using on a new artificial equation in the governing mathematical model. The moving boundary is the zero-level set of an auxiliary field, $\phi(x)$, defined over the domain of interest. The level set method is applied to identify and track an interface inside a continuum, commonly for AM process in the microscale.

It has enough potential to expand to the macro scale simulations. The interface is defined by an isovalue, $\phi = 0$ of $\phi(x, t)$, which is the signed distance function to the interface at any location and instant in the continuum. The discontinuity between inert gas and the consolidated workpiece is treated with a Heaviside function. Then the field value of the whole domain is calculated by a mixture law. After one step of deposition, the level set function must be updated as the interface has moved. An overall schematic picture is shown in Figure 10.

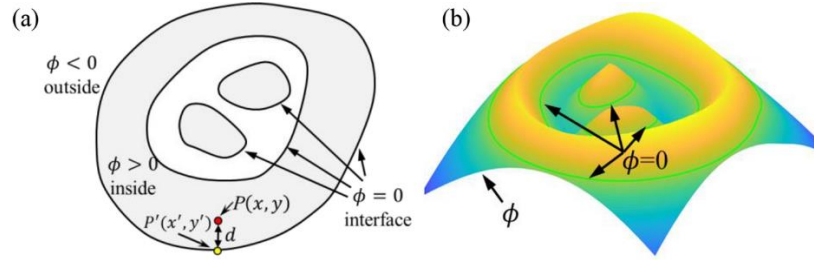


Figure 10 Implicit function $\phi(x)$, its boundaries, and distance function. a cross section and boundary, b surface and boundary [72].

3.3.3. Volume of fluid method for the free boundary

Several methods have been previously used to approximate free boundaries in finite difference and finite element numerical simulations. The fractional volume of fluid (VOF) method is a simple but powerful method, that is more flexible and efficient than other methods for treating complicated free boundary configurations. In the micro-scale simulation of additive manufacturing, the VOF method is often used to track the position and shape of the molten pool surface [73][74] by solving the scalar transportation function for the volume fraction of fluid whose value varies between 0-1. The volume fraction represents the intrinsic materials (powder, consolidated workpiece segments, inert gas). The interface between different materials is captured artificially by a threshold volume fraction, as shown in Figure 11. Both the LSM and the VOF separate the space into two domains continuously, but the LSM has the merit to define more precisely the location and curvature of the interface, although it does not guarantee the conservation of mass [75].

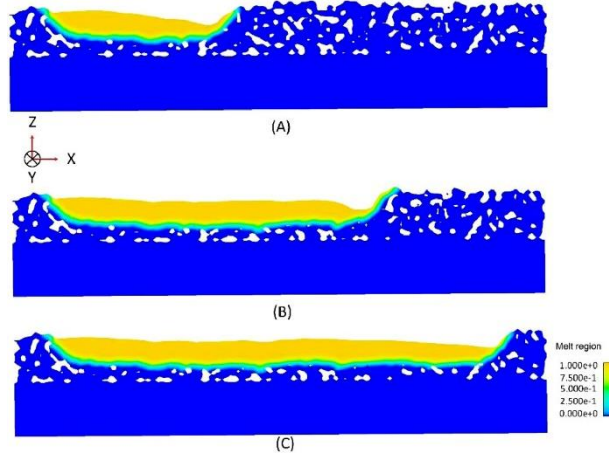


Figure 11 The formation of the melt pool resorting to the VOF formulation in various time steps [75].

3.3.4. Finite cell method

The basic concepts of the finite cell method (FCM) are briefly summarized for linear elasticity. A detailed description of the FCM can be found, for example, in [76]. The FCM embeds a physical domain Ω_{phy} into a fictitious domain Ω_{fict} forming an extended domain Ω_U , as illustrated in Figure 12. As with the procedures in traditional FEM, the problem solved by the finite cell method should be first described mathematically, resorting to a weak formulation. The weak formulation is modified by extending integrals over the union Ω_U domain of the physical domain Ω_{phy} and the fictitious domain Ω_{fict} . Some terms in the weak formulation of FCM are multiplied by a scalar field α that is defined as a discontinuous indicator function, referring to the geometric description of the physical domain Ω_{phy} and the fictitious domain Ω_{fict} . With the help of an adaptive mesh technique, it is possible to simulate the complex geometry of the workpiece constructed by additive manufacturing. The boundary conditions in the FCM, both Neumann in Γ_N or Dirichlet in Γ_D , are difficult to treat and they must be handled in a particular manner, because the boundaries of the physical domain $\partial\Omega_{phy}$ typically do not coincide with that of the extended union domain.

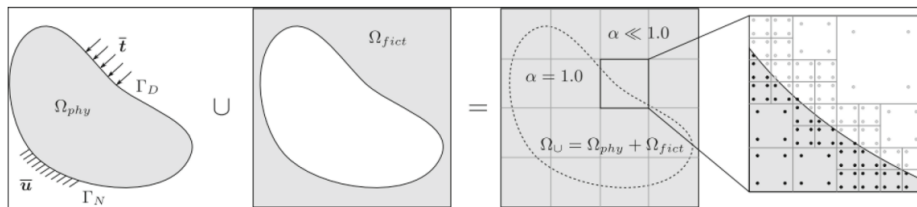


Figure 12 The concept of the finite cell method. The integration on the cut cell requires special quadrature rules – here indicated by a composed integration on a quadtree reconstruction [76].

3.3.5. Phase field method

Historically moving boundary problems have been challenging from a computational point of view, but more recently, a number of new computational methods have been developed to solve them numerically. The FCM [77], VOF [78] and LSM [71] methods are based on the tracking or capturing of sharp interfaces. The front-tracking algorithm can be used in conjunction with adaptive mesh refinement near the interface, but it is difficult to apply it to dynamic interfaces that undergo complicated topological changes. VOF methods have the advantage of conserving mass by explicitly tracking for each cell. Still, the reconstruction of interfaces from volume fractions and calculation of associated geometric quantities, such as the interface curvature, is not straightforward. The level set method, on the other hand, can handle complex geometries effectively. It provides a robust framework for representing and evolving interfaces. However, without additional techniques such as volume-of-fluid or front tracking approaches [79], [80] or adaptive mesh refinement [81], the level set method may encounter challenges related to mass loss or gain. In contrast, the diffuse-interface models, such as the phase-field approach, do not require explicit computing of the moving interface. The approach, initially developed by van der Waals in the 1800s and by Cahn and Hilliard [88] in the 1950s, is based on the concept of a diffuse interface that can be defined in terms of a density, structure or composition field (i.e., a phase field) that changes smoothly from one phase to the other over an interface zone with a non-zero width, ω (Figure 13(a-b)). In this manner, numerical difficulties associated with the boundary conditions at the sharp interfaces are avoided, and no explicit interface tracking/capturing is required. The phase field is transported locally with the velocity of the interface, and deformation of the phase field is restored by diffusive relaxation (Cahn–Hilliard[82]) of conservative phase fields or direct relaxation (Allen–Cahn[83]) of non-conservative fields. Initially proposed for the applications such as the solidification of pure melts [84,85], the phase field approach has been used to simulate a wide variety of interface dynamics phenomena, including two-phase Navier–Stokes flow [86], crack propagation [87]. However, in most applications, the phase field equations are only used to circumvent the difficulty of tracking sharp interfaces, where the equations and/or their associated parameters do not directly represent the physics of the interfaces. Phase field methods have also been used in conjunction with particle models such as smoothed particle hydrodynamics (SPH) and dissipative particle dynamics (DPD), either to calculate forces based on a free energy functional [88], or more precisely locate complex boundaries [89].

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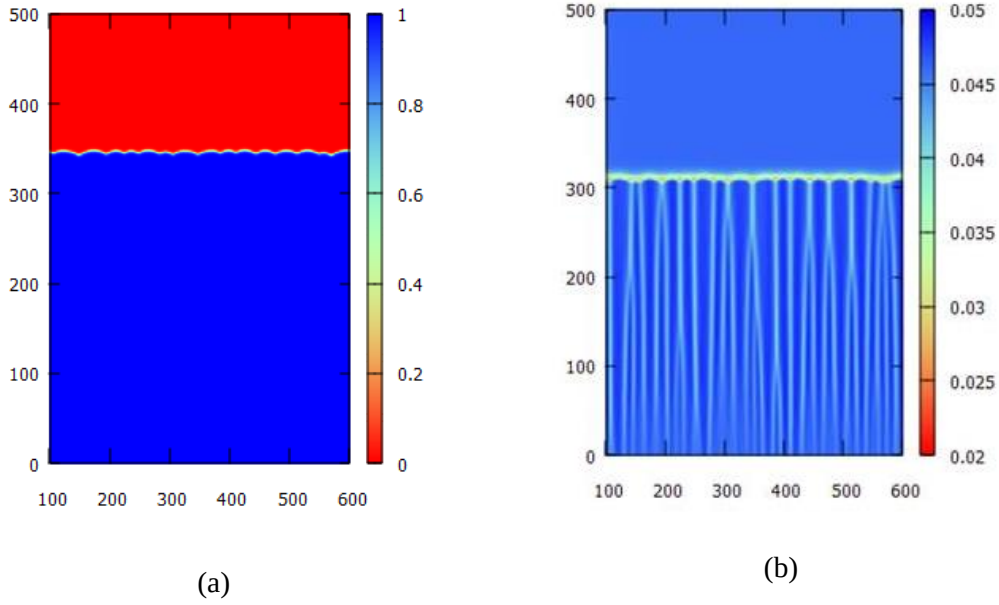


Figure 13 Phase transition, (a): Solidification frontier by Allen-Cahn, (b): Concentration field during solidification (binary Ni-Nb) by Cahn-Hillard phase field models.

3.4. Numerical solution for phase change and latent heat

Two crucial aspects of macroscale AM modeling are phase change and latent heat effects. Specifically, a systematic formulation of phase fraction variables is proposed, relying on either temperature or enthalpy-based interpolation schemes. Moreover, the following section reviews two well-known schemes for the numerical treatment of latent heat: the apparent capacity (AC) and the heat integration (HI) schemes.

3.4.1. Apparent heat capacity

One of the most straightforward approaches to capturing the effects of latent heat is the so-called apparent capacity (AC) method. The basic idea is that phase change takes place within a finite temperature interval of width $2d$, $[T - d; T + d]$. Throughout this work, the temperature bounds confining this regularized phase change interval is assumed taking $T_s = T - d$ and $T_l = T + d$, as the solidus and liquidus temperature for the mushy zone phase. As simple as the AC method may be, it suffers from one major drawback: an accurate representation of the phase change constraint, i.e., the choice of a small phase change interval $2d$, yields large values and gradients of the function for the specific heat capacity, which is not only challenging for numerical solution schemes (e.g., nonlinear solvers) but also prone to large-time integration errors. In this case, the absorbed or released enthalpy during a phase change, and thus the overall energy balance of the phase change problem are only captured with low accuracy [90].

3.4.2. Heat integration method

Hu and Argyropoulos [91] presented a more advanced method called the heat integration (HI) method. The basic concept relies on proposing an alternative interpretation of the heat integration method as an augmented Lagrange constraint enforcement scheme, which is explained in [92] in detail. One of the main drawbacks of this classical heat integration approach is that heat can be transferred from any stream to another as long as it flows from higher temperature intervals to lower ones, leading to impractical scenarios in which heat is recovered over long distances.

Chapter 4

Theoretical basis for additive manufacturing simulation

4.1.Introduction

Additive manufacturing (AM) poses a complex multi-field coupling problem, involving intricate interactions between thermal, mechanical, and metallurgical fields. The challenge lies in solving these three distinct fields on the same scale (whether length or time) and effectively coupling them together. Additionally, the description of additive manufacturing varies across different scales, adding to the complexity. In this study, we focus on the macro scale of numerical simulation, aiming to extend its applicability to industrial scenarios, particularly for predicting distortions. To address the tradeoff between different phases and boundary conditions for the material phases (powder, liquid, solid), we opt to separate the computational domain into distinct continuum subdomains. Utilizing the phase field model, we can effectively capture the melting effect of metal during deposition, while also considering the phase-change effects in both thermal and mechanical analyses. The following section presents a logically structured hierarchical computational stage that enriches the different thermal, mechanical, and metallurgical domains. This approach enables a comprehensive understanding of the additive manufacturing process, paving the way for more accurate predictions and practical applications.

4.2.Mathematical description of thermal elastoplastic phase field model

4.2.1. Kinetics of the thermo-mechanical formulation

This section presents two different uncoupled and fully coupled, thermodynamically-consistent phase-field thermo-mechanical modeling approaches for AM. Consider a solid domain $\Omega \in \mathbb{R}^3$. At each material point $\mathbf{x} \in \Omega$ and time $t \in [0, \tau]$, the thermomechanical problem is described by the following field variables:

$$\mathbf{u}: \begin{cases} \Omega \times \tau \rightarrow \mathbb{R}^{d3} \\ (\mathbf{x}, t) \rightarrow \mathbf{u}(\mathbf{x}, t) \end{cases}, \quad T: \begin{cases} \Omega \times \tau \rightarrow \mathbb{R} \\ (\mathbf{x}, t) \rightarrow T(\mathbf{x}, t) \end{cases}, \quad \phi: \begin{cases} \Omega \times \tau \rightarrow [0,1] \\ (\mathbf{x}, t) \rightarrow \phi(\mathbf{x}, t) \end{cases} \quad (4.1)$$

where $\mathbf{u}$, T and ϕ respectively represent the displacement vector, temperature and phase-field variables. The phase changing setting in the present work considers $\phi = 0$ and $\phi = 1$ as the soft (liquid) powder and hard (solid) powder states, respectively, while $0 < \phi < 1$ represents the in-between mushy phase zone. Following the infinitesimal deformation theory, whereby $\boldsymbol{\varepsilon} = \nabla_s \mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u})$, the total strain tensor $\boldsymbol{\varepsilon}$ can be additively decomposed into elastic ($\boldsymbol{\varepsilon}^e$), plastic ($\boldsymbol{\varepsilon}^p$) and thermal ($\boldsymbol{\varepsilon}^{th}$) strain tensors, such that

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p + \boldsymbol{\varepsilon}^{th} \quad (4.2)$$

4.3.Free energy function

The thermo-elastoplastic problem is described by the following set of independent state variables

$$\mathcal{V} = \{\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \alpha, T, \nabla T, \phi, \nabla \phi\} \quad (4.3)$$

where $\alpha, T, \nabla T, \phi, \nabla \phi$ are equivalent plastic strain, temperature, temperature gradient, phase field and phase field gradient, respectively. The free energy density function per unit volume can be written as

$$\psi(\mathcal{V}) = \psi^e + \psi^p + \psi^{th-e} + \psi^{th} + \psi^\phi \quad (4.4)$$

where $\psi^e, \psi^p, \psi^{th-e}, \psi^{th}$ and ψ^ϕ are the elastic, plastic, thermo-elastic, pure thermal and phase-field energy contributions. The free energy terms can be detailed as [93]:

$$\left\{ \begin{array}{l} \psi^e = \frac{K}{2} \varepsilon_v^2 + \mu \boldsymbol{\varepsilon}_d^e : \boldsymbol{\varepsilon}_d^e, \end{array} \right. \quad (4.5a)$$

$$\left\{ \begin{array}{l} \psi^p = \sigma_y \alpha + \frac{1}{2} H \alpha^2, \end{array} \right. \quad (4.5b)$$

$$\left\{ \begin{array}{l} \psi^{th-e} = -3K\xi \varepsilon_v (T - T_0), \end{array} \right. \quad (4.5c)$$

$$\left\{ \begin{array}{l} \psi^{th} = c \left[(T - T_0) - T \ln \left(\frac{T}{T_0} \right) \right], \end{array} \right. \quad (4.5d)$$

$$\left\{ \begin{array}{l} \psi^\phi = f(\phi, T) + \frac{\epsilon_\phi^2}{2} \|\nabla \phi\|^2. \end{array} \right. \quad (4.5e)$$

where K, μ are, respectively, the bulk and shear moduli, $\varepsilon_v = \text{tr}(\boldsymbol{\varepsilon}^e)$ is the volumetric strain and $\boldsymbol{\varepsilon}_d^e = (\boldsymbol{\varepsilon}^e - \frac{1}{3} \varepsilon_v \mathbf{I})$ is the deviatoric elastic strain tensor. Within the plastic energy term, σ_y and H are the initial yield stress and hardening modulus respectively. The remainder of the parameters are ξ , the thermal expansion coefficient, T_0 the reference temperature, c the heat capacity per unit volume and $\mathbf{I}$ a second order identity tensor. In the expression of the phase field energy, ψ^ϕ , the bulk free energy contribution $f(\phi, T)$ is added to the interfacial energy density as the local dissipation term, consisting of the phase-field gradient term and its coefficient ϵ_ϕ , which will be further explored in the next section. The time rate of the free energy can be obtained as follows:

$$\dot{\psi} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} : \dot{\boldsymbol{\varepsilon}} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} : \dot{\boldsymbol{\varepsilon}}^p + \frac{\partial \psi}{\partial \alpha} : \dot{\alpha} + \frac{\partial \psi}{\partial T} \dot{T} + \frac{\partial \psi}{\partial \nabla T} \cdot \nabla \dot{T} + \frac{\partial \psi}{\partial \phi} \dot{\phi} + \frac{\partial \psi}{\partial \nabla \phi} \cdot \nabla \dot{\phi}. \quad (4.6)$$

By using the divergence theorem, the last term in the above equation can be written as:

$$\frac{\partial \psi}{\partial \nabla \phi} \cdot \nabla \dot{\phi} = \text{div} \left(\dot{\phi} \frac{\partial \psi}{\partial \nabla \phi} \right) - \text{div} \left(\frac{\partial \psi}{\partial \nabla \phi} \right) \dot{\phi}. \quad (4.7)$$

In order to obtain thermodynamically consistent constitutive relations governing the coupled thermomechanical problem, the second law of thermodynamics (entropy inequality) is used which

can be interpreted in the form of the following generalized Clausius–Duhem inequality [94] per unit volume as:

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\psi} - s\dot{T} - \frac{1}{T}\mathbf{q} \cdot \nabla T \geq 0. \quad (4.8)$$

where $\boldsymbol{\sigma}$ is Cauchy stress tensor and s and $\mathbf{q}$ are the entropy density and the heat flux vector, respectively. Substituting equations (4.6) and (4.7) into the inequality in equation (4.8) reads

$$\begin{aligned} \left(\boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} \right) : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} \dot{\boldsymbol{\varepsilon}}^p - \frac{\partial \psi}{\partial \alpha} \\ : \dot{\alpha} - \left(s + \frac{\partial \psi}{\partial T} \right) \dot{T} - \frac{\partial \psi}{\partial \nabla T} \cdot \nabla \dot{T} - \left(\frac{\partial \psi}{\partial \phi} - \operatorname{div} \frac{\partial \psi}{\partial \nabla \phi} \right) \dot{\phi} \\ - \operatorname{div} \left(\dot{\phi} \frac{\partial \psi}{\partial \nabla \phi} \right) - \frac{1}{T} \mathbf{q} \cdot \nabla T \geq 0. \end{aligned} \quad (4.9)$$

which must be held for any arbitrary thermodynamic process. In light of Colman's thermodynamical framework in [95,96], the following equilibrium equations can be derived:

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} = K(e - \xi(T - T_0))\mathbf{I} + 2\mu\boldsymbol{\varepsilon}_d^e, \quad (4.10)$$

$$s = -\frac{\partial \psi}{\partial T} = 3K\xi e + \operatorname{cln}\left(\frac{T}{T_0}\right) + \rho L\left(\frac{1}{T_M}\right)p(\phi). \quad (4.11)$$

with T_M , ρ and L as the material melting temperature, density and latent heat of fusion per unit volume, respectively. It also can be established that the free energy does not depend on the temperature gradient, such that

$$\frac{\partial \psi}{\partial \nabla T} = \mathbf{0}, \quad (4.12)$$

Furthermore, one can establish that $\operatorname{div}\left(\dot{\phi} \frac{\partial \psi}{\partial \nabla \phi}\right) = 0$. The volume integration over the domain Ω can be returned as the following surface integral using the Gauss integral theorem:

$$\int_{\Omega} \operatorname{div}\left(\dot{\phi} \frac{\partial \psi}{\partial \nabla \phi}\right) d\Omega = \int_{\partial\Omega} \left(\dot{\phi} \frac{\partial \psi}{\partial \nabla \phi}\right) \cdot \mathbf{n} d\partial\Omega. \quad (4.13)$$

where $\mathbf{n}$ is the outward unit normal vector to the boundary surface $\partial\Omega$. This implies the following Neumann type boundary condition

$$\dot{\phi} \frac{\partial \psi}{\partial \nabla \phi} \cdot \mathbf{n} = 0. \quad (4.14)$$

As for the remaining part of equation (4.9), the following dissipative inequalities are established

$$-\frac{1}{T} \mathbf{q} \cdot \nabla T \geq 0, \quad (4.15)$$

$$-\left(\frac{\partial \psi}{\partial \phi} - \operatorname{div} \frac{\partial \psi}{\partial \nabla \phi} \right) \dot{\phi} \geq 0, \quad (4.16)$$

$$\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} : \dot{\boldsymbol{\varepsilon}}^p - \frac{\partial \psi}{\partial \alpha} \dot{\alpha} \geq 0. \quad (4.17)$$

The thermal dissipation in equation (4.15) is based on the Fourier's law, $\mathbf{q} = -\kappa \nabla T$, which assumes that heat transfers from warmer to colder material spots for a positive heat conductivity parameter κ . The energetic driving force conjugate to the internal variable α can be derived in correspondence with the dissipative inequality (4.17) as follows

$$q_\alpha = -\frac{\partial \psi}{\partial \alpha} = -H\alpha. \quad (4.18)$$

With the above definition at hand, the mechanical dissipation can be described using the reduced Clausius-Planck inequality as

$$D = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p + q_\alpha \dot{\alpha} \geq 0. \quad (4.19)$$

4.4. Phase Field models

In connection with the temperature-related phase change of the metallic material, the phase-field related energy function $\frac{\delta \psi^\phi}{\delta \phi}$ (equation (4.5e)) is expressed in terms of a bulk free energy contribution $F(\phi, T)$ and the interfacial energy terms. Thus, in analogy to the thermodynamically consistent approach in [97] and following the Ginzburg Landau theory [97], the global potential energy function F over a spatial domain Ω is expressed as the summation of the interfacial energy term as:

$$F(\phi, T) = \int_{\Omega} [f(\phi, T) + l^2 |\nabla \phi|^2] d\Omega \quad (4.20)$$

with l being the gradient-energy coefficient that influences the width of the diffusive zone. In phase field formulations, the diffusive zone refers to the region near the sharp interface where the phase transition occurs. It represents the gradual transition between two distinct phases or materials. The width of the diffusive zone determines the smoothness of the interface and affects the accuracy of the phase field simulation. At equilibrium, from the variational derivative of F

$$\frac{\delta F}{\delta \phi} = \frac{\delta \psi^\phi}{\delta \phi}, \quad (4.21)$$

the following restriction results:

$$\frac{\delta \psi^\phi}{\delta \phi} = \frac{\partial f}{\partial \phi} - \epsilon_\phi^2 |\nabla \phi|^2 = 0. \quad (4.22)$$

Herein, $f(\phi, T)$ depends on the phase field model used. In the following section, two models will be presented.

4.4.1. Allen-Cahn PF method

The interfacial diffusion is a time-dependent process and, therefore, the evolution of the phase-field parameter can be suitably described by the time derivative of a non-conserved variable η in the form of the Allen-Cahn equation

$$\frac{\partial \eta}{\partial t} = -M \left[\frac{\partial F}{\partial \eta} \right], \quad (4.23)$$

with F being the free energy functional that, in its general form, contains the local and gradient terms for conserved and non-conserved field variables. The above equation can be equivalently written as:

$$\frac{\partial \phi}{\partial t} = -M \left[\frac{\partial f}{\partial \phi} - \frac{l^2}{2} \nabla^2 \phi \right], \quad (4.24)$$

The interface mobility parameter M is a positive value which can be defined based on [98]

$$M = \frac{\mu_\phi T_M}{6\delta\rho L}. \quad (4.25)$$

with μ_ϕ and δ as the interface kinetic coefficient and the interface width, respectively. Based on [98], a common form of the free energy density of the system can be defined as:

$$f(\phi, T) = Wg(\phi) + \Theta(T)p(\phi), \quad (4.26)$$

In the FE implementation the element size has to be chosen sufficiently smaller than the value of δ in order to achieve the necessary resolution at the solid-liquid interface. Furthermore, in equation (4.22), the phase-field gradient coefficient ϵ_ϕ is equivalent to the length scale defining the width of the diffusive interface of width l ; W is the interfacial energy barrier, with $W = 3 \frac{\omega}{\delta}$ where ω is the surface tension and $\Theta(T)$ is the thermal driving force for the phase changing problem as follows

$$\Theta(T) = \rho L \left(\frac{T_M - T}{T_M} \right), \quad (4.27)$$

Equation (4.26) shows a competition between an energy barrier at the interface of the solid and liquid phases and the difference of the free energy terms associated with these phases around the melting point. Following the above relations, the free energy associated with the phase-field variable previously defined in equation (4.5e) can be rewritten as

$$\psi^\phi = Wg(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p(\phi) + \frac{l^2}{2} \|\nabla\phi\|^2, \quad (4.28)$$

The choice of $g(\phi)$ and $p(\phi)$, respectively a double well potential and an interpolating function, are arbitrary. In the present work, the functions from [98] were employed:

$$g(\phi) = \phi^2(1 - \phi)^2, \quad (4.29)$$

$$p(\phi) = \phi^3(6\phi^2 - 15\phi + 10). \quad (4.30)$$

Taking into account the above relations and equation (4.24), the evolution of the phase field variable is given by

$$\dot{\phi} = -M \left[W g'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) - \text{div}(l^2 \nabla \phi) \right]. \quad (4.31)$$

4.4.2. Wang Phase Field method

Based on Wang et al. [99] a different form of equation (4.26) (free energy density of the system) can be defined as:

$$f(\phi, T) = T \left(- \int_{T_M}^T \frac{e_L(\zeta)}{\zeta^2} d\zeta - (p(\phi) - 1) \Phi(T) + \frac{1}{4a} g(\phi) \right). \quad (4.32)$$

In the previous equation $\Phi(T)$ is the thermal driving force for the phase changing problem between solid and liquid and is defined as follows:

$$\Phi(T) = \int_{T_M}^T \frac{L}{\zeta^2} d\zeta, \quad (4.33)$$

and the integral term is defined as

$$\int_{T_M}^T \frac{e_L(\zeta)}{\zeta^2} d\zeta = [e_L(T_M) - c T_M] \left(\frac{1}{T} - \frac{1}{T_M} \right) + c \ln\left(\frac{T}{T_M}\right) \quad (4.34)$$

where e_L is the internal energy of the liquid phase and c is volumetric heat capacity.

The evolution of the phase field variable is given by

$$\dot{\phi} = -\frac{1}{\tau} \left[\frac{1}{4a} g'(\phi) - \Phi(T) p'(\phi) - \text{div}(l^2 \nabla \phi) \right]. \quad (4.35)$$

where $\tau = (6\sqrt{2}\delta L/\mu_\phi T_M^2)$, $a = (\sqrt{2}\delta T_M/12\omega)$ are parameters related to the interface mobilities and interfacial energy barrier.

4.5. Governing balance equations

In the absence of external forces, the balance of the linear momentum reads:

$$\nabla \sigma = 0. \quad (4.33)$$

The stress tensor, dual to the elastic strain tensor ϵ^e , can be written as

$$\sigma = \frac{\partial \psi}{\partial \epsilon^e} = \mathbb{C}^e \epsilon^e, \quad (4.34)$$

Based on equation (4.2), the above relation can be alternatively written as

$$\sigma = \mathbb{C}^e (\epsilon - \epsilon^p - \epsilon^{th}), \quad (4.35)$$

with $\mathbb{C}^e$ as the fourth-order elastic stiffness tensor and the thermal strain expressed by

$$\epsilon^{th} = \xi(T - T_0)\mathbf{I}, \quad (4.36)$$

Aimed at obtaining the governing energy balance equation and the entropy evolution, we start from first law of thermodynamics that prescribes the conservation of internal energy as:

$$\dot{E} = \sigma : \dot{\epsilon} - \nabla \cdot \mathbf{q} + Q. \quad (4.37)$$

where E is the specific internal energy and Q is the external heat supply per unit volume.

Using the Legendre transform the internal energy can be converted into the sum of the free energy and entropy-temperature potentials, $E = \psi + sT$, that in its rate form can be written as

$$\dot{E} = \dot{\psi} + s\dot{T} + \dot{s}T, \quad (4.38)$$

Based on the inequality given in equation (4.14), the rate of the free energy described in equation (4.6) can be rewritten as

$$\dot{\psi} = \sigma : \dot{\epsilon} - D - s\dot{T} + \left[\left(\frac{\partial \psi}{\partial \phi} - \text{div} \frac{\partial \psi}{\partial \nabla \phi} \right) \dot{\phi} \right]. \quad (4.39)$$

4.5.1. Allen-Cahn Phase Field model for the fully coupled approach

Using equations (4.26) and (4.39) alongside the internal energy rate forms outlined in equations (4.37) and (4.38), one can write

$$T\dot{s} = D - \left[Wg'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) - \text{div}(l^2 \nabla \phi) \right] \dot{\phi} - \text{div} \mathbf{q} + Q, \quad (4.40)$$

In parallel to the above equation and given that $s = -\frac{\partial \psi}{\partial T}$, the time rate of the entropy density can be derived, using the chain rule, as

$$\begin{aligned} \dot{s} = & -\frac{\partial(\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - D)}{\partial T} - \frac{\partial^2 \psi}{\partial T^2} \dot{T} \\ & - \frac{\partial}{\partial T} \left[Wg'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) - \text{div}(l^2 \nabla \phi) \right] \dot{\phi}, \end{aligned} \quad (4.41)$$

Replacing the equation (4.41) into (4.40), yields

$$c\dot{T} = D + W^{ep} - W^\phi - \text{div} \mathbf{q} + Q, \quad (4.42)$$

with

$$c = -T \frac{\partial^2 \psi}{\partial T^2}, \quad (4.43)$$

$$W^{ep} = T \frac{\partial(\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - D)}{\partial T}, \quad (4.44)$$

$$W^\phi = \left[\rho L \left(\frac{T}{T_M} \right) p'(\phi) + Wg'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) - \text{div}(l^2 \nabla \phi) \right] \dot{\phi}. \quad (4.45)$$

where c is the volumetric heat capacity and W^{ep} and W^ϕ are the contributions related to the elastoplastic and phase-field problems.

4.5.2. Wang PF model for decoupled approach

Equation (4.35) may be combined with energy density equations (4.46, 4.47) as follows:

$$e = c_s(\varphi)T + p(\phi)[L_0 + [c_L - c_s(\varphi)](T - T_M)] \quad (4.46)$$

$$c_s(\varphi) = (1 - \varepsilon_0(1 - \varphi))c_d \quad (4.47)$$

The temperature variation of energy density term, $\frac{de}{dT}$, is the heating capacity function, The heat capacity function, represented by $c_s(\varphi)$ incorporates the dense heat capacity (c_d) while considering the initial porosity effect (ε_0). Therefore, equation (4.42) can be transformed into equation (4.45) to account for the presence of a heat source in the uncoupled based on the Wang PF formulation.

$$\rho \frac{de}{dT} \frac{dT}{dt} + \nabla \cdot [k(\varphi) \cdot \nabla T] - s(\mathbf{x}, t) = 0 \quad (4.48)$$

In equation (4.49), the term $k(\varphi)$ represents the thermal conductivity, which is a combination of the thermal conductivities of the powder phase (k_p) and the mixture of dense or molten (k_d) material phases. The thermal conductivity can be expressed as a function of the solid k_s and liquid k_L states.

$$k(\varphi) = (1 - \varphi)k_p + \varphi k_d \quad (4.49)$$

$$k_d = (1 - \phi)k_s + \phi k_L \quad (4.50)$$

Additive manufacturing involves a direct energy source to melt powder layers that condense and then solidify on the substrate or prior layers. The laser path can be defined by the laser center coordinate on the surface of the substrate, $s(\mathbf{x}, t)$, as a function of time. The laser moves simultaneously with spreading powder from nozzles throughout the deposition zone. In order to distinguish the phases during the process, two state variables, φ and ϕ , are defined so that $0 \leq \varphi, \phi \leq 1$. The first state variable φ is the consolidation parameter, so that when $\varphi = 1$ the material is fully dense, while when $\varphi = 0$ the material is in a powder state. The second state variable ϕ is the phase parameter so that $\phi = 0$ refers to a fully solid region and $\phi = 1$ refers to a molten phase. Figure 14 illustrates the combination of various phases in metal additive manufacturing process. In section 4.7, the state variables' function is explained in a more detailed procedure.

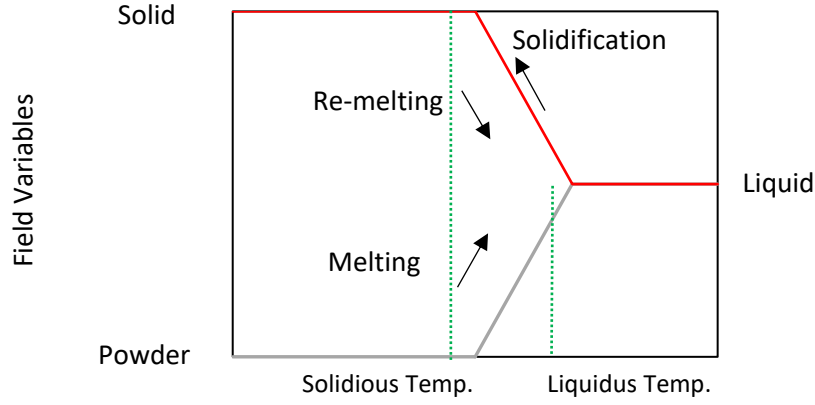


Figure 14 Diagram of field state phase changes between powder/liquid/solid states.

4.6. Classical J_2 plasticity model

In what follows, a brief overview of associative rate-independent J_2 plasticity theory using isotropic hardening law is given which is employed herein to allow for plastic deformations within the constitutive model. The standard yield function using von Mises criterion is given by

$$f_y(\boldsymbol{\sigma}_d, q^\alpha, T) := \sigma_{eq} - Y(\alpha), \quad (4.51)$$

where $Y(\alpha) = \sigma_Y - q^\alpha$ with σ_Y as the material yield stress and $\sigma_{eq} = \sqrt{3J_2} = \left(\frac{3}{2}\boldsymbol{\sigma}_d : \boldsymbol{\sigma}_d\right)^{\frac{1}{2}}$ is the equivalent von Mises stress, in which $\boldsymbol{\sigma}_d = \boldsymbol{\sigma} - \frac{1}{3}tr(\boldsymbol{\sigma})\mathbf{I}$ is the deviatoric stress tensor. The rate of the stress tensor can be given, according to equation (4.35), as

$$\dot{\boldsymbol{\sigma}} = \mathbb{C}^e(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^p + \dot{\boldsymbol{\varepsilon}}^{th}), \quad (4.52)$$

where $\mathbb{C}$ is the elasticity tensor.

The rate of the plastic strain can be defined via the associative flow rule

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda} \frac{\partial f_y}{\partial \boldsymbol{\sigma}}, \quad (4.53)$$

where $\dot{\lambda}$ is the plastic multiplier and $\frac{\partial f_y}{\partial \boldsymbol{\sigma}}$ indicates the direction of the plastic strain increment.

Using the chain rule, the time derivative of the yield function reads

$$\dot{f}_y = \frac{\partial f_y}{\partial \boldsymbol{\sigma}} : \dot{\boldsymbol{\sigma}} + \frac{\partial f_y}{\partial \dot{q}} \dot{q}, \quad (4.54)$$

Then, the accumulated (equivalent) plastic strain can be written as

$$\bar{\boldsymbol{\varepsilon}}^p = \left(\frac{2}{3} \boldsymbol{\varepsilon}^p : \boldsymbol{\varepsilon}^p \right)^{\frac{1}{2}}, \quad (4.55)$$

The plastic consistency parameter must satisfy the Kuhn-Tucker conditions given by

$$\dot{\lambda} \geq 0 \quad , \quad \dot{\lambda} f_y = 0 \quad , \quad f_y \leq 0. \quad (4.56)$$

4.7. Irreversible phase change of powder

The history variable field φ , so-called consolidation as introduced previously, is utilised to prevent the return of the solidified phase to powder, ensuring that the following condition is always met:

$$\varphi(\mathbf{x}, t + \Delta t) \geq \varphi(\mathbf{x}, t) \quad (4.57)$$

where $\varphi(\mathbf{x}, t + \Delta t)$ is the phase field variable for consolidation in the current time increment while $\varphi(\mathbf{x}, t)$ denotes the value of the consolidation on the previous increment. Furthermore, φ is defined as the maximum of $\phi(\dot{\mathbf{t}})$ over the time interval $[0, t]$:

$$\varphi = \max\{\phi(\dot{\mathbf{t}})\} \quad (4.58)$$

$$\dot{\mathbf{t}} \in [0, t]$$

where $\phi(\dot{\mathbf{t}})$ represents the current value of the phase field function during melting/solidification

4.8. Metallurgical phase fraction prediction by Johnson-Mehl-Avrami (JMA) model

In additive manufacturing of a metallic part, the residual stress and strains could be bred by the solid phase transformation during the high-frequency heating and cooling cycles. The metallurgical properties of different metal solid phases impact the mechanical or thermal behavior during additive manufacturing. The field of a material's volume fraction, which is a macroscopic scalar field, cannot be used to describe the metallurgical microstructure of metal crystals. Still, it

is important to forecast or measure the solid phase transformation during the cyclic heating and cooling in AM process. The solid phase transformation of steel or titanium alloy depends kinetically on the cooling rate of the AM process. According to different mechanisms, the solid phase transformation can be classified into two kinds: martensitic transformation and diffusional transformation. In the following section, the proposed strategy allows for transitioning from isothermal to non-isothermal conditions, enabling the justification of rapid cooling phenomena in the AM process. In AM thermo-metallurgical simulation procedures, the temperature evolution history of the thermal field serves as the input data for the metallurgical simulation.

4.8.1. Isothermal Johnson-Mehl-Avrami (JMA) model

The standard JMA equation is widely used in modeling of the temporal evolution of phase transformation ξ under isothermal conditions [100] using equation (4.59).

$$\xi = 1 - \exp(-kt^n) \quad (4.59)$$

where k is the temperature dependent kinetic constant, t is time, and n is the Avrami exponent representing the transformation behavior. These kinetics parameters including nucleation, growth and impingement stages describe the transformation mechanism. The value of n is greater for interface-controlled growth rather than for diffusion-controlled growth. In the kinetic theory developed based on Gibb's formalism the steady-state rate of nucleation (J), which is equal to the number of nuclei formed per unit time per unit volume, is expressed according to the classical nucleation theory as equation (4.60) [101][102]

$$J = ZN_0\beta^* \exp\left(-\frac{\Delta G^*}{k_B T}\right) \quad (4.60)$$

The variables in this equation are explained in the following paragraphs.

Z represents the Zeldovich factor [103], which can be expressed in detailed form as :

$$Z = \left(\frac{a^6 \Delta G_v^4}{64\pi^2 k_B T \gamma_s^3 V_m^4} \right)^{1/2} \quad (4.61)$$

in which a is a lattice constant of the matrix phase (β), ΔG_v is the bulk thermodynamic driving force for nucleation of the precipitate (α) in matrix phase (β), γ_s is the interfacial energy between the phases in the matrix (β) and the precipitate (α), V_m represents the molar volume of the matrix phase (β). N_0 is the nucleation site density and can be rewritten as,

$$N_0 = N_A/V_m \quad (4.62)$$

where N_A is the Avogadro constant.

β^* is the atomic attachment rate which is represented as

$$\beta^* = \frac{16\pi\gamma_s^2 V_m^2 D c_\beta^e}{\Delta G_v^2 a^4 (c_\alpha^e - c_\beta^e)} \quad (4.63)$$

where D represents the diffusion coefficient and c_α^e and c_β^e are the equilibrium solute compositions of the α and β phases ($\beta \rightarrow \alpha$). As explained before, V_m represents the molar volume of the matrix phase (β). Finally, ΔG^* is the free energy cost of the nucleus at the top of the nucleation barrier, k_B is Boltzman constant, and T is the temperature. Besides, the growth rate u of the diffusion-controlled growth of a particle can be written as equation (4.65) [104].

$$u = \sqrt{2 \frac{c_0 - c_\beta^e}{c_\alpha^e - c_\beta^e} D} \quad (4.64)$$

in which c_0 is the mean solute concentration in the matrix (β). The nucleated particle(s) volume is/are $V_p = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi(u^3(t - \tau)^{1.5})$ in which the radius r of the spherical particle during the incubation time (τ) is assumed as $r = u(t - \tau)^{0.5}$. When new particles nucleate in the untransformed region at a rate, independent of the coordinates, within the time period $d\tau$, the number of particles nucleated is given by $N_p = (1 - \xi).J.d\tau$. Therefore, the variation of the phase fractions through this time period can be expressed as equation (4.66).

$$d\xi = N_p V_p = \frac{4}{3}\pi(u^3(t - \tau)^{1.5}).J.(1 - \xi) d\tau \quad (4.65)$$

The detailed formulation of equation (4.59) can be derived by integration as below,

$$\xi = 1 - \exp\left(\frac{-8\pi}{15} \cdot u^3 \cdot J \cdot t^{2.5}\right) \quad (4.66)$$

From the expanded form of equation (4.59) to equation (4.66), the value of the reaction rate constant (k) is $\frac{-8\pi}{15}u^3J$ and the Avrami exponent (n) equals 2.5.

4.8.2. Non-isothermal JMA model by incremental formulation approach

The JMA model for phase transformations considers the mechanisms of continuous and random nucleation under isothermal conditions, as described in section 4.8. However, for the highly non-isothermal condition of solidification in DED, the JMA model needs to be modified. In the references [105][106][107], the application of the principle of additivity for time increments has been successfully documented to describe the kinetics of phase transformations in case studies for titanium alloys and microstructure modeling for welding processes. To address the non-isothermal condition, an incremental calculation of the transformations during a small-time step, known as the fictive time, is necessary. This fictive time is much shorter than the time constant of the transformation. The additive fictive time, denoted as t_A , is added to each time step to represent the time required to reach the current phase fraction if the entire transformation occurred isothermally at the current temperature. Therefore, ξ is employed to express the extent of the reaction, and f represents the phase fraction during non-isothermal analysis. In the first isothermal time step, which is shown in Figure 15(a) at $T = T_0$, the reaction extent in equation (4.60) can be rewritten as equation (4.68).

$$\xi(t_1) = 1 - \exp(-k(T_0) \cdot (t_1 - t_0)^n) \quad (4.68)$$

meanwhile $(t_1 - t_0)$ is the first fictive time increment

For the first fictive time step, where the lack of reaction is isothermal and the additivity principle applies, the α phase fraction $f^\alpha(t_1)$ can be calculated using the equilibrium phase fraction $f^{\alpha e}(T_0)$ obtained from Thermo-Calc graphs, as shown in equation (4.69)

$$f^\alpha(t_1) = f^{\alpha 0} + (f^{\alpha e}(T_0) - f^{\alpha 0}) \cdot \xi(t_1) \quad (4.69)$$

The next fictive additional time is added incrementally with equation (4.70).

$$t_{A1} = \left(-\frac{\ln \left(1 - \frac{f^\alpha(t_1) - f^{\alpha 0}}{f^{\alpha e}(T_1) - f^{\alpha 0}} \right)}{k(T_1)} \right)^{1/n} \quad (4.70)$$

For the next isothermal step $(t_2 - t_1)$, as shown in Figure 15 (a), in the T_1 , the reaction calculation should be multiple to the reaction term as equation (4.71).

$$\xi(t_2) = 1 - \exp(-k(T_1) \cdot (t_2 - t_1 + [t_{A1}])^n) \quad (4.71)$$

With respect to equation (4.72), the expanded phase fraction for the next time step is rewritten as equation (4.72) and illustrated in Figure 15 (b).

$$f^{\alpha}(t_2) = f^{\alpha 0} + (f^{\alpha e}(T_1) - f^{\alpha 0}) \cdot \xi(t_2) \quad (4.72)$$

Remark:

This computational trend repeats for all arbitrary isothermal time steps to cover all temperature profile points. Leveraging MATLAB capabilities, an algorithm was implemented to derive the temperature from FEM simulation and the database from Thermo-Calc. The kinetic mechanism and its parameters should be collected to formulate the reaction rate constant $k(T)$ and the Avrami exponent.

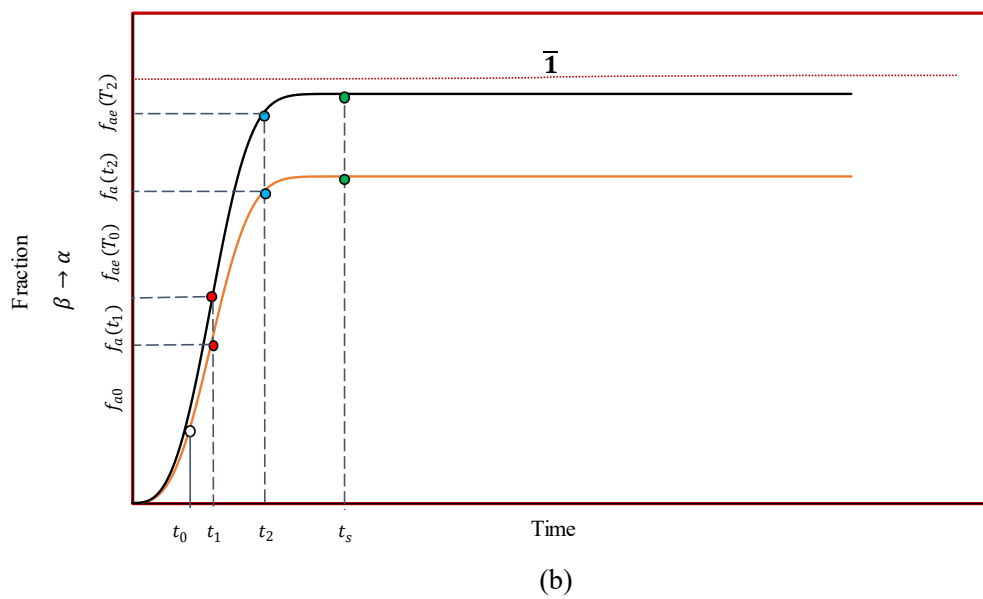
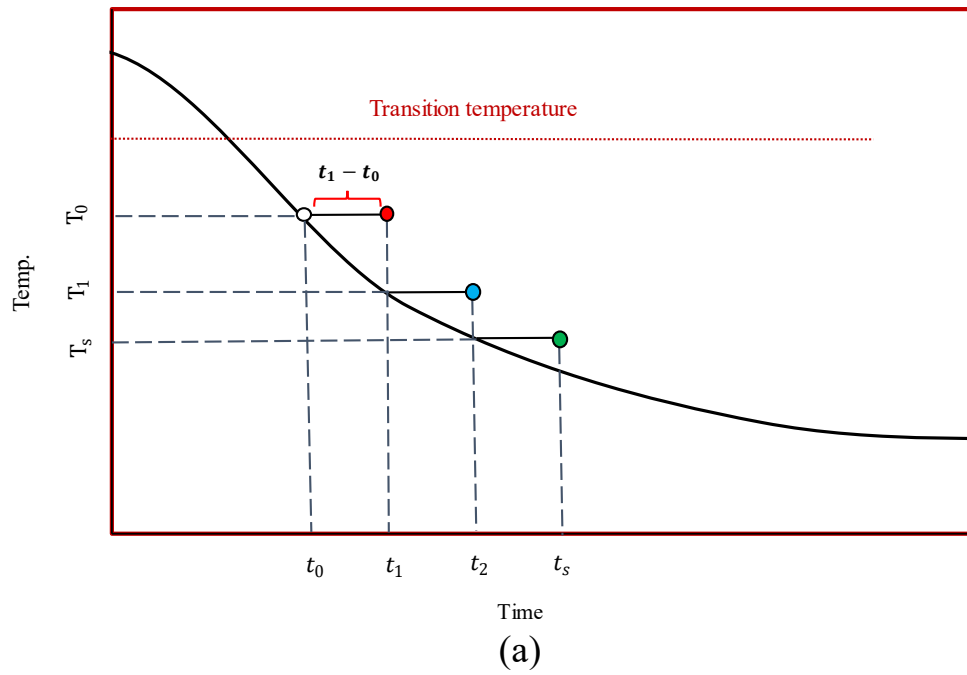


Figure 15 Implementation of non-isothermal phase fraction using the fictive additionally time increment (a): temperature profile in cooling stage, (b): transition from phase fraction of equilibrium to non-isothermal condition.

4.9. Metallurgical phase evolution prediction by Phase field modelling

Inconel 625 is a complex alloy composed of approximately twelve or more components. Upon undergoing thermal aging, several distinct phases can be observed in Inconel 625, namely γ'' , δ , Laves, MC, M₆C, and M₂₃C₆ carbides. Due to its relatively low levels of aluminum and titanium, Inconel 625 is unable to form the L12-ordered γ' phase that is present in many other nickel-base superalloys (such as Inconel 718). For this study, the focus is on intragranular precipitation, and therefore only the strengthening γ'' phase is taken into account. In order to capture the essential characteristics of the precipitation process while conserving computational resources, a pseudo-ternary (Ni-Al_x-Nb_y) CALPHAD thermodynamic database designed for Ni-based superalloys [108] was utilized. Within this database, Al_x is treated as a weighted summation of all elements that contribute to the formation of the γ' phase (namely, aluminum and titanium), and is represented by Al*. Similarly, Nb_y is considered as a weighted summation of all elements that form the γ'' and δ phases (namely, niobium and tantalum), and is represented by Nb*. The system is depicted by two composition fields, χ_{Al} and χ_{Nb} . The γ'' phase, which is a tetragonal structure located within the cubic γ matrix, features an orientation relationship of $\{100\}\gamma''//\{100\}\gamma$ and $[001]\gamma''//\langle 100\rangle\gamma$, resulting in the appearance of three orientation variants with distinct $\{100\}$ habit plane. To ensure accuracy in the 3D phase-field simulations, all three orientation variants of the γ'' phase were taken into account. For each variant of γ'' , two antiphase domains were introduced. The inclusion of antiphase domains for each variant of γ'' in the simulations serves to decrease the likelihood of coalescence events between identical variants during the growth and coarsening stages. In the simulations, γ'' is represented using three order parameters denoted as $\{\eta_1, \eta_2, \eta_3\}$ which correspond to the three variants $\{\pm 1, 0, 0\}$, $\{0, \pm 1, 0\}$, and $\{0, 0, \pm 1\}$, respectively. The two antiphase domains of the same variant are represented by +1 and -1. When $\eta_j = 0$, it corresponds to the matrix phase, while $0 < |\eta_j| < 1$ corresponds to the γ/γ'' interface. The temperature-dependent total free energy functional for the single crystal system will be discussed in detail in the following sections, regarding both isothermal and non-isothermal aging conditions.

4.9.1. Phase-field representation of a mixture of γ/γ'' phases

The multi-phase field model can be used to describe phase transformations in alloys with arbitrary numbers of product phases, variants, and chemical components. The order parameter in this model is an N-component vector, where N represents the total number of product phases/variants. For a given product phase-variant m , it is represented by $\eta_{v=m} = 1$ and $\eta_{v \neq m} = 0$.

The parent (matrix) phase is described when all components of the order parameter are zero, i.e., $\vec{\eta} = 0$. The standard formulation considers various energy contributions, including interfacial energy f_{int} , chemical free energy f_{chem} , gradient energy f_{grad} , due to the inhomogeneous distribution of the order parameters, and the elastic energy f_{el} associated with the phase transformations and mismatch between the matrix and phases of the system.

$$F = \int dV (f_{int} + f_{chem} + f_{grad} + f_{el}) \quad (4.73)$$

4.9.2. Interfacial energy density

The interfacial energy density contribution f_{int} is considered as:

$$f_{int} = \omega^{\gamma''} \sum_{i=1}^3 [\eta_i^2 (1 - |\eta_i|)^2] + \alpha \sum_{i=k}^4 \sum_{i \neq k}^4 \eta_i^2 \eta_k^2 \quad (4.74)$$

where $\omega^{\gamma''} = 1.49 \times 10^8$ (J/m³), characterizing the free energy humps (barriers) between the matrix and three precipitate phases, respectively. In order to ensure that only the order parameter corresponding to the given phase is non-zero, the parameter α is chosen to be sufficiently large, and is chosen here to be 1.07×10^{11} (J/m³).

4.9.3. Chemical free energy

The chemical free energy of the system is given by the sum of the Gibbs free energy of different phases and the energy variation due to structural changes. Mathematically, it can be expressed as follows,

$$f_{chem} = \frac{1}{V_m} \left[\left(1 - \sum_{j=1 \dots 4} h(|\eta_j|) \right) f^{\gamma} + \left(\sum_{j=1 \dots 3} h(|\eta_j|) f^{\gamma''} \right) \right] \quad (4.75)$$

Herein, $h(|\eta_j|) = (|\eta_j|)^3 [6|\eta_j|^2 - 15|\eta_j| + 10]$ is the interpolation function, $V_m = 1 \times 10^{-5}$ (m³/mol) is the molar volume, and f^γ , $f^{\gamma''}$ are the free energies of the coexisting phases as a function of Al and Nb concentrations. These terms are approximated by parabolic functions using the second derivatives of the matrix phase free energy with respect to Al and Nb concentrations at equilibrium as the coefficients, i.e.

$$f^\gamma = [C_{Al}(\chi_{Al}^\gamma - \chi e_{Al}^\gamma)^2 + C_{Nb}(\chi_{Nb}^\gamma - \chi e_{Nb}^\gamma)^2] \quad (4.76)$$

$$f^\delta = [C_{Al}(\chi_{Al}^\delta - \chi e_{Al}^\delta)^2 + C_{Nb}(\chi_{Nb}^\delta - \chi e_{Nb}^\delta)^2] \quad (4.78)$$

In above formulations, $C_{Al} = 4.0 \times 10^5$ (J/mol) and $C_{Nb} = 9.5 \times 10^5$ (J/mol) are obtained from the pseudo-ternary thermodynamic database [108]. According to the phase diagram which is presented in [108], the equilibrium compositions $(\chi e_{Al}^\gamma, e_{Nb}^\gamma) = (1.61 \times 10^{-2}, 7.23 \times 10^{-3})$ and $(\chi e_{Al}^\delta, \chi e_{Nb}^\delta) = (7.27 \times 10^{-4}, 1.96 \times 10^{-1})$ can be calculated as well. Besides, as the δ (stable phase) and γ'' (metastable) phases have similar equilibrium compositions, the free energy of the metastable $f^{\gamma''}$ phase is formulated as:

$$f^{\gamma''} = f^\delta + \Delta f \quad (4.79)$$

The free energy difference near the equilibrium composition of the δ phase, $\Delta f = 1548.5$ (J/mol), was obtained from the pseudo-ternary database [108].

4.9.4. Gradient energy with cross terms

The gradient energy term in the free energy functional describes the energy penalty that arises due to the inhomogeneous distribution of phase-field variables near interfaces as:

$$f_{grad} = \sum_{i=2} \frac{\kappa_i}{2} (\nabla \chi_i)^2 + \sum_{j=1 \dots 4} \frac{\kappa_j}{2} (\nabla \eta_j)^2 \quad (4.80)$$

where κ_i, κ_j is the gradient energy coefficients of specific phases. Herein, $\kappa_i = 0$ and κ_j can be described by using the barrier values from Equation 4.74, interfacial energy $(\sigma^j(T))$ of that phase at temperature T and its interface thickness (l_0) to the following forms:

$$\sigma^j(T) = \frac{\sqrt{\kappa_j \cdot \omega^j}}{3\sqrt{2}} \quad (4.81)$$

$$2l_0 = 2.2\sqrt{2}\sqrt{\frac{\kappa_j}{\omega^j}} \quad (4.82)$$

4.9.5. Elastic free energy

Regarding Equation 4.73, the structural transformation during precipitation generates strains that may substantially change the free energy. The elastic energy in a general case is expressed as:

$$f_{el} = \frac{1}{2} \sum_{ijkl} C_{ijkl}(T) e_{ij} e_{kl} \quad (4.83)$$

Elastic tensor $C_{ijkl}(T)$ (see Figure. 16) and strain tensor e_{ij} fields are interpolated between known values for each phase:

$$C_{ijkl}(T) = \left(1 - \sum_j h(|\eta_j|)\right) C_{ijkl}^{\gamma} + \left(\sum_j h(|\eta_j|) C_{ijkl}^j\right) \quad (4.84)$$

$$e_{ij} = \varepsilon_{ij} - \left(\sum_j h(|\eta_j|) \varepsilon_{ijkl}^j\right) - \delta_{ij} \varepsilon_{th} \quad (4.85)$$

Here ε_{ij}^j are the components of transformation strain tensor for the phase, ε_{th} represents thermal strain. The strain tensor is calculated by using the displacement fields u_i as $\varepsilon_{ij} = 1/2 (\partial u_i / \partial x_j + \partial u_j / \partial x_i) + \bar{\varepsilon}_{ij}$ and the stress tensor is calculated as: $\sigma_{ij} = \partial f_{el} / \partial \varepsilon_{ij}$. For a macroscopically stress-free system, $\bar{\varepsilon}_{ij}$ is chosen such that all stress components average to zero.

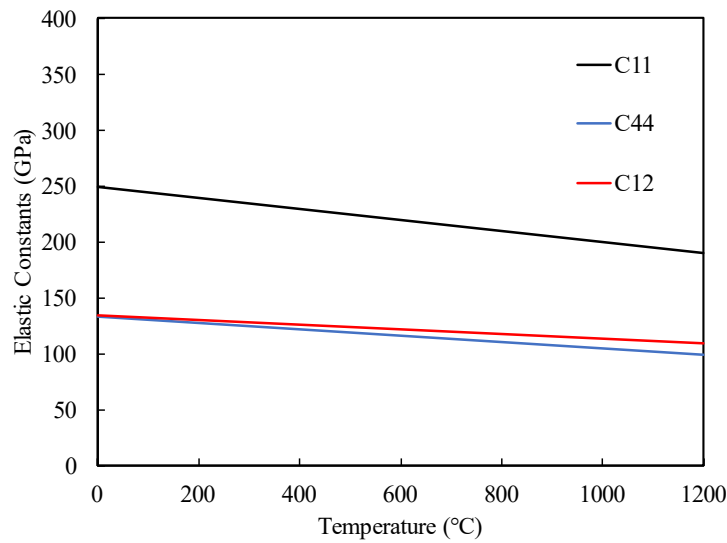


Figure 16 The elastic constants for the γ phase in Inconel 625 can be described by the following linear equation as a function of temperature: $C_{11} = 249.5 - 0.0495T$, $C_{12} = 132.7 - 0.0284T$, $C_{44} = 133.9 - 0.0204T$. where C_{11} , C_{12} , and C_{44} are the elastic constants in GPa, and T is the temperature in Kelvin. These equations were derived by Wang et al. [109] based on their experimental data [109].

To satisfy the free energy term, during a cubic-to-cubic transformation, the stress-free transformation strain (SFTS) for the $\gamma \rightarrow \gamma''$ transformation is explained in Equations 4.86-4.88 [109][110]:

$$\varepsilon^{\gamma''}_1 = \begin{bmatrix} 0.0286 & 0 & 0 \\ 0 & 0.0067 & 0 \\ 0 & 0 & 0.0067 \end{bmatrix}; \quad (4.86)$$

$$\varepsilon^{\gamma''}_2 = \begin{bmatrix} 0.0067 & 0 & 0 \\ 0 & 0.0286 & 0 \\ 0 & 0 & 0.0067 \end{bmatrix}; \quad (4.87)$$

$$\varepsilon^{\gamma''}_3 = \begin{bmatrix} 0.0067 & 0 & 0 \\ 0 & 0.0067 & 0 \\ 0 & 0 & 0.0286 \end{bmatrix}. \quad (4.88)$$

The eigenstrain coefficient for γ'' is typically in the range of -0.1% to -0.2%, while for γ it is typically in the range of -0.05% to -0.1%. These values can vary depending on the specific alloy composition and processing conditions. The negative eigenstrain coefficient for these phases is beneficial for the high-temperature performance of nickel-based superalloys, as it can help to stabilize the material against creep deformation and improve its mechanical strength.

4.9.6. Governing kinetic equations

The transformation kinetics of the system is described by the standard set of phase field equations that are coupled with the multi-component diffusion equations. The non-conserved phase parameter, η_j , is expressed as Equation 4.89 based on Allen-Cahn phase field model.

$$\frac{\partial \eta_j}{\partial t} = -L \frac{\delta F}{\delta \eta_j} \quad (4.89)$$

L is the kinetic coefficient for structural evolution. The value of L is selected to ensure diffusion-controlled growth of the precipitates. $L = \frac{L^* D}{E_0 l_0^2}$ in which that $L^* = 10$ for all range of temperature. Herein, $l_0 = 0.5$ (nm), $E_0 = 2.5$ (GPa), reference energy density. The concentration of Al and Nb as two conserved variables, χ_{Al} and χ_{Nb} , can be uttered as Equations 4.90 and 4.91;

$$\frac{\partial \chi_{Al}}{\partial t} = V_m^2 \nabla \cdot (M_{Al} \nabla \tilde{\mu}_{Al}) \quad (4.90)$$

$$\frac{\partial \chi_{Nb}}{\partial t} = V_m^2 \nabla \cdot (M_{Nb} \nabla \tilde{\mu}_{Nb}) \quad (4.91)$$

where M_i ($i = Al^*, Nb^*$) are the thermos chemical mobilities of Al^* and Nb^* , respectively. The mobilities can be estimated as $M_i = D_i/V_m(\partial^2 f^r/\partial \chi_i^2)$, where $D_i = D_0 \exp(Q/RT)$ ($i = Al^*, Nb^*$) are the temperature dependent diffusivities of Al and Nb. $D_{0Nb} = D_{0Al} = 8.8 \times 10^{-5} (m^2/s)$ and $Q_{Nb^*} = 295 (kJmol^{-1})$, $Q_{Al^*} = 325 (kJmol^{-1})$ are diffusion activation energies.

4.9.6.1. Kim-Kim-Suzuki (KKS) model of interface treatment

The KKS model [111–114] is used to treat the interphase interfaces in order to decouple interfacial energy from the width of the interfaces. This is critical to simulate microstructural features at micrometer length scales. The equal chemical potential condition within an equilibrium interface is guaranteed by the following equations:

$$\tilde{\mu}_{Al} = \frac{\partial f^r}{\partial \chi_{Al}^r} = \frac{\partial f^{r''}}{\partial \chi_{Al}^{r''}} = 2V_m^{-1} C_{Al}(\chi_{Al}^r - \chi_{eAl}^r), \quad (4.92)$$

$$\tilde{\mu}_{Nb} = \frac{\partial f^r}{\partial \chi_{Nb}^r} = \frac{\partial f^{r''}}{\partial \chi_{Nb}^{r''}} = 2V_m^{-1} C_{Nb}(\chi_{Nb}^r - \chi_{eNb}^r). \quad (4.93)$$

As parabolic functions are used to describe the free energy near the equilibrium compositions of the phases, the first derivatives of the free energy with respect to concentration in the above equations are linear functions of concentration. Thus, numerical implementations of Equations (4.76) and (4.78) are straightforward.

Chapter 5

Proposed workflow with commercial software, codes, FEM implementations'

5.1.Introduction

This chapter presents a proposed workflow for simulating the additive manufacturing (AM) process using commercial software and codes, with a specific focus on the Direct Energy Deposition (DED) process with ABAQUS and the Powder Bed Fusion (PBF) process with MOOSE. The AM process involves complex interactions between thermal, mechanical, and metallurgical fields, making its numerical simulation challenging. The workflow begins by developing a numerical framework for simulating a single layer of the AM process (cladding) and gradually expands to model the entire part, incorporating more complexity. The hierarchical approach enriches the model, capturing a broader range of phenomena that occur during the AM process. The incorporation of the ABAQUS software enables the accurate analysis of thermal and mechanical responses, allowing for the optimization of process parameters and evaluation of part quality. Furthermore, the use of AM Modeler, a user-friendly plugin, facilitates the simulation of SLM and DED processes. The MOOSE framework with the libMesh finite element library and adaptive mesh refinement is employed to model the PBF process, considering the intricate physical phenomena involved. The proposed workflow aims to provide a comprehensive understanding of the AM process, enabling accurate predictions and insights into the final part's properties and behavior, thereby enhancing the efficiency and effectiveness of the AM process.

5.2.Direct Energy Deposition Process with ABAQUS

In this section, the primary objective is to establish a workflow for simulating the additive manufacturing (AM) process using the ABAQUS software. The AM process poses specific challenges and constraints when applying the finite element method, and this chapter aims to address and overcome them. To accomplish this, we start by developing a numerical framework that focuses on a single layer of the AM process, commonly referred to as cladding. Simulating this smaller scale can lay the foundation for a more comprehensive and accurate model.. Building upon the cladding simulation, we then expand the workflow to encompass larger scales, such as manufacturing the entire part. This hierarchical approach allows us to enrich the model, incorporating more complexity and capturing a broader range of phenomena that occur during the AM process. Figure 17 illustrates the progression of the workflow, showcasing the step-by-step refinement from one scale to another. Starting with the cladding simulation, we gradually incorporate additional layers and features to simulate the manufacturing process at the part scale. This hierarchical workflow ensures a comprehensive understanding of the AM process, enabling accurate predictions and insights into the final part's properties and behavior. By following this workflow and utilizing the capabilities of the ABAQUS software, we aim to provide a robust and reliable simulation framework for additive manufacturing. This framework will aid in optimizing

process parameters, predicting part quality, and ultimately enhancing the overall efficiency and effectiveness of the AM process.

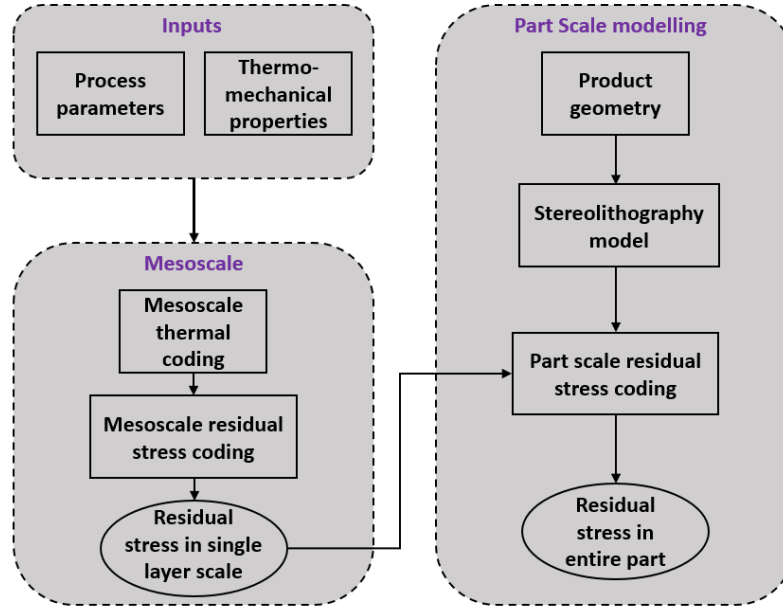


Figure 17 Schematic of multiscale modeling linkage in using predicted results from mesoscale model for part scale residual stress/strain calculation.

5.2.1. Reconstruction of 3D model at layer size

The basic procedure of the AM process, specifically for DED or PBF/SLM, follows a similar sequence of steps. The initial stage involves acquiring the geometry of the part to be additively manufactured, typically in STL (stereolithography) format. The STL file represents the surface geometry of the part through a collection of triangular facets. Once the STL file is available, the next step is to discretize the part geometry into slices. This process divides the three-dimensional model into a series of two-dimensional layers, which will be successively built during the AM process. Following the slicing stage, the specific scan parameters from the AM machine need to be incorporated into an input file. These parameters include laser power, beam locations, beam size diameter, scan speed, and travel distance. To accomplish this, a G coder is employed to translate the scan parameters into machine-readable instructions. In this case, the ReplicatorG-0040 software [115] can serve as the G coder tool. To prepare the G code file for utilization within finite element analysis (FEA) software, a Python script is commonly employed. This script converts the G code file into a format that the FEA software can effectively interpret. The resulting file format is typically *.inp, which represents the trajectory of the laser heat source and the path of material deposition during the AM process. The generated *.inp file can then be utilized as an input in software such as ABAQUS, which is a widely used FEA software package. ABAQUS

utilizes the trajectory information to model the interaction between the laser heat source and the material, enabling the analysis of thermal and mechanical responses, including temperature distribution, residual stresses, and deformation. Incorporating the AM machine's scan parameters into the simulation workflow and utilizing the STL and G code files makes it possible to simulate the additive manufacturing process accurately. This allows for optimising process parameters, evaluating part quality, and identifying potential issues or defects in the manufactured components.. The use of the *.inp files as inputs in ABAQUS provides a comprehensive representation of the laser heat source trajectory and material deposition path, enabling detailed analysis and understanding of the AM process.

5.2.2. Element activation strategy

The key point in ABAQUS is the toolpath-mesh intersection module [116]. The module finds intersections between the finite element spatial discretization (meshes) and the scan path created from a python script. As the simulation of the AM process requires numerical interpretation in terms of automated element activation and related heat input in time and space, the ABAQUS event series module was utilized herein to prescribe the imposed tool path and process conditions. Once the AM printing process is translated into event series format, the newly introduced tool path-mesh intersection module automatically computes the information required for the thermal and structural FEM analysis, including the element activation and relevant thermal and structural boundary conditions for each given time step as Figure 18. SLM processes typically utilize coarse meshes with “point” approaches to interpret the heating process and “infinite lines” for the separate process of the recoater element activation. DED process simulation generally uses a fine mesh with “box” approaches to simultaneously deposit and heat the newly activated elements [117]

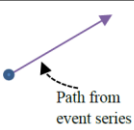
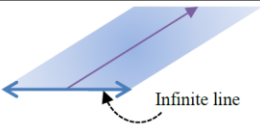
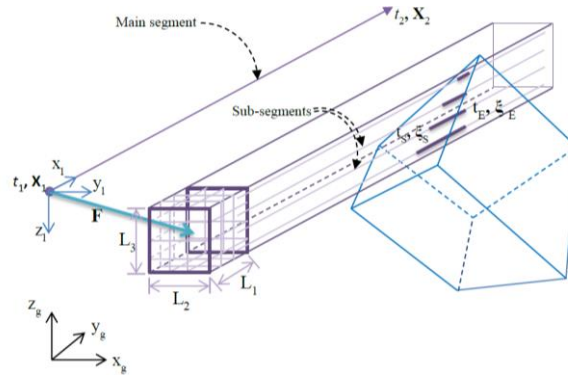
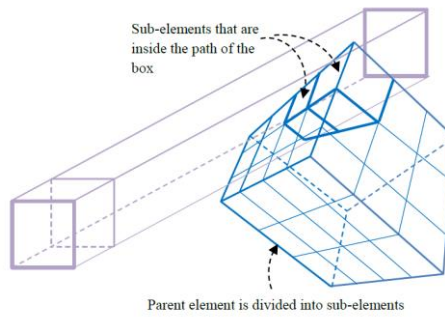
Shape	Point	Infinite Line	Box
Schematic			
Machine tool examples	Point lasers for coarse meshes	Recoater in powder-bed fabrication	Material deposition nozzle in polymer extrusion, wire-feed, laser blob for fine meshes, etc.

Figure 18 Intersection shapes for event series interpretation in the ABAQUS mesh intersection module.

Intersections of a box toolpath and a mesh can be computed using two different algorithms, namely, the sub-segment and the sub-element approaches, as Figure 19 (a, b), respectively. The technique utilized in this study is sub-segment implementation.



(a)



(b)

Figure 19 (a) Box-line toolpath mesh intersection using the sub-segment and (b) sub-element approaches [117].

At the very first iteration, all the elements belonging to the build-up pool are “passivated”[117]. All those passivated elements then automatically stay in the initial temperature field until activation is requested, as shown in Figure 20. When a toolpath comes across a set of elements, the thermal-physical properties for the liquid phase, by taking to account the degree of consolidation, are automatically assigned with the correct values of the activated elements. Likewise, the degree of consolidation is related directly to the history of the material phase change parameter, as described in Chapter 5, section 5.2.3. After the heat source is applied to the elements, the material properties change to whether the mushy melt-dense or fully dense material states with respect to their temperature history. Once the status of those elements is changed to active, the element set external surface is updated to apply the new boundary conditions, which are treated as a combined boundary condition with a modified heat transfer coefficient.

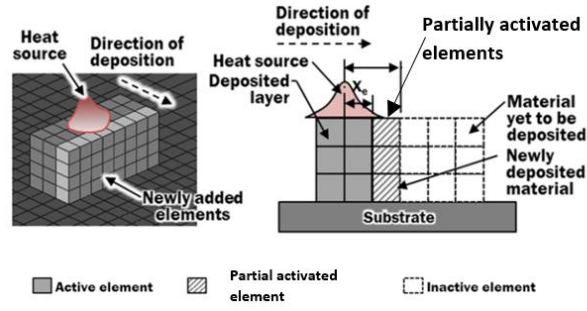


Figure 20 Element activation strategy scheme.

5.2.3. Heat source modelling for DED

It is important to establish an appropriate heat source model of laser deposition simulations since the heat source not only influences the geometries of melt pools but might also impact the mechanical performance of final products. Heat source models used in our simulations are typically assumed as the following two-dimensional exponentially decaying expression, which is schematically represented in Figure 21. [118][119] regarding equation (5.1). The movement of the heat source is implemented with an event series replicating exactly the movement of the scanning strategy [120], and the respective element birth technique follows the laser trajectory

$$s(x, y, z, t) = \frac{fP}{\pi r_l^2} \exp\left(-f \frac{x^2 + (y - v_y \cdot t)^2}{r_l^2}\right) f(z) \quad (5.1)$$

$$f(z) = \frac{\beta}{H} \exp\left(-\frac{|z|}{H}\right)$$

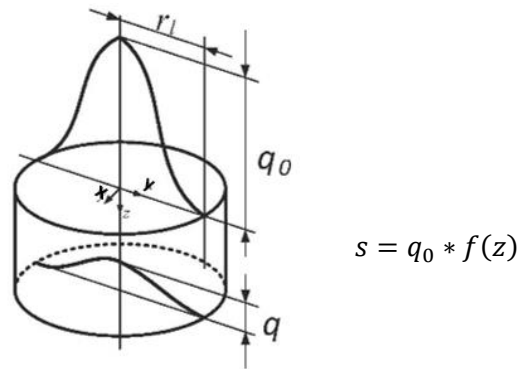


Figure 21 The schematic of heat source with exponentially decaying method.

where P is the laser power, f is the distribution of power factor, r_l is laser beam radius corresponding to the distance between the beam center and the point with coordination (x, y) , $\beta \sim 0.65$ is average laser energy absorptivity of a material affected by the wavelength of the laser, H is the laser penetration depth as the material properties and $f(z)$ is the absorptivity profile

function of heat source in Z direction. The laser energy density reduced to both horizontal and depth directions at the center of the laser spot. Figure 22 illustrates the schematic profile of power density with respect to the distribution factor.

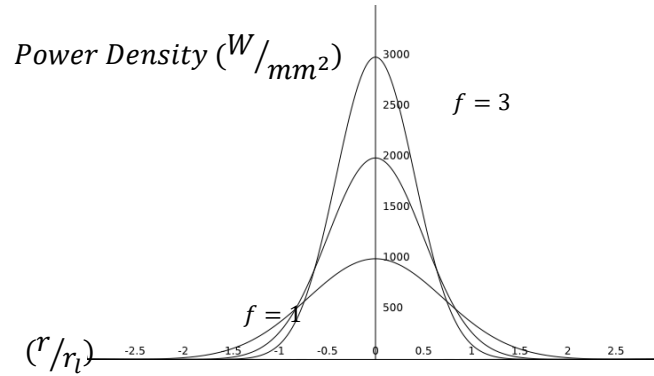


Figure 22 The powder density distribution with a laser power of 2 kW according to the distribution factors.

5.2.4. AM Plugin application

In this thesis, the presented physical phenomenon in Chapter 4, is implemented using an user-subroutine, which generally requires considerable expertise. Additionally, recent versions of ABAQUS offer a new plugin tool, AM Modeler, which provides a relatively new and user-friendly method for performing additive manufacturing process simulations. The AM Modeler tool combines user subroutines internally and provides a graphical user interface (GUI) for ease of use. In our previous research, we executed the whole process of selective laser melting (SLM) and direct energy deposition (DED) taking advantage of the aforementioned AM plugin [121][122]. Herein, for the track-scaled simulation, only user-subroutines can steer the process simulations, while in the multi-track scale, for element activation strategy, the provided event series in AM plugin is used. The event series can be imaged as a combination of path and amplitude. Time (t) and position (x, y, z) are mandatory columns in an event series for defining the time and space variation of the event path, and user-defined dependent variables can also be added to prescribe the corresponding amplitude. In our simulations, two event series with input files are defined for respectively simulating the deposition of raw powder layers and the movement of laser p relatively.

5.3. Powder Bed Fusion Process with MOOSE

The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a high-performance, open-source, C++ finite element toolkit developed at Idaho National Laboratory [123,124]. It is designed to assist domain scientists and engineers in creating customizable, high-quality tools for

multi-physics simulations. The MOOSE framework itself does not contain code for simulating any specific physical application, but it comes with several physics' "modules" tailored to solving problems such as heat conduction, phase field, and solid/fluid mechanics (Figure 23). MOOSE widely uses Jacobian-free Newton-Krylov (JFNK) as a core mathematical principle behind the numerical framework to solve the non-linear system of equations. This approach is a combination of Newton's method and the Krylov subspace method, which allows for the rapid production of new simulation tools by modularizing physics expressions into "Kernels." By using physics-based preconditioning and enabling to solve the systems implicitly and fully coupled, MOOSE provides the users with great flexibility, even when dealing with problems with large variations in time scales. Underneath MOOSE is the libMesh finite element framework developed by the CFDLab at the University of Texas in Austin [125]. The libMesh provides a set of utilities for massively parallel finite element-based computations, including mesh I/O, a finite element library, and interfaces to solver packages. Utilizing the interfaces in libMesh provides MOOSE, and subsequently, the applications built using MOOSE, a significant amount of flexibility, including the ability to swap out solver libraries and to utilize diverse large-scale parallel computing resources.

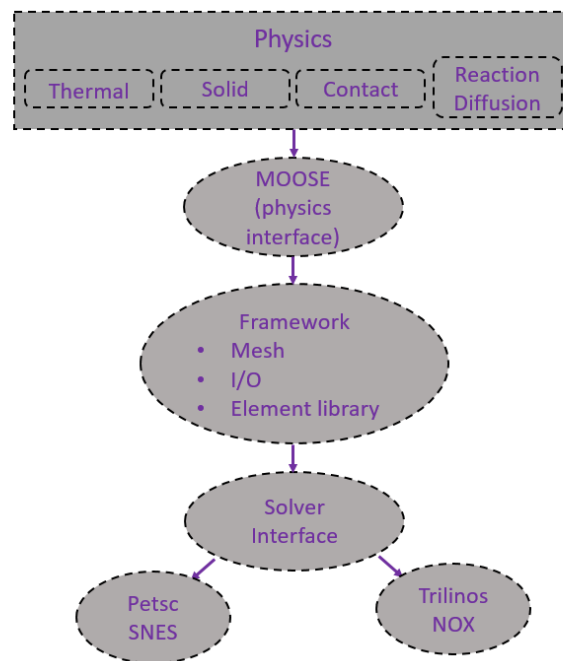


Figure 23 MOOSE structure graph.

5.3.1. Coupled Multiphysics and Multi scale medium

Parts fabricated with the powder bed fusion (PBF) process frequently encounter defects such as lack of melting and layer delamination due to an insufficient understanding of the complicated physical phenomena involved, e.g., mass and energy transport, material phase changes, and

microstructure evolution. In the PBF process, melt pools are created as the moving heat source melts the powder. The choice of process parameters can heavily influence the characteristics of these melt pools. Many physical phenomena in PBF manufacturing occur in a very short time and at a small scale, i.e., several milliseconds and micrometers, making it challenging, if not impossible, to experimentally monitor the entire manufacturing process. Therefore, physically-accurate modeling of this manufacturing process can play a vital role in the qualification of components and materials. In PBF, the physical phenomena are interrelated. Multiphysics-based numerical models are well suited to investigate the influence of process characteristics such as powder layer melting, temperature distribution, solidification, and phase changing. The physics of fully coupled thermo-mechanical phenomena in the melt pool domain can be represented by a phase-field model based on the Allen-Cahn equation, ensuring tracking of the interface in the phase-changing melt pool medium.

5.3.2. LibMesh finite element library with adapted mesh refinement (AMR)

The libMesh finite element library was created by Benjamin Kirk [125] as part of his doctoral work to provide an alternative to the deal.II library [126], with a focus on adaptive mesh refinement (AMR) capabilities for unstructured meshes including triangles and tetrahedra. The library supports a range of geometric elements and finite elements, including traditional Lagrange, hierarchical bases, Clough-Toucher macroelements, and Nedgelec elements of the first type. The libMesh offers parallel distributed meshes and fully supports distributed parallel adaptive mesh refinement, allowing it to be scaled up to tens of thousands of cores and run on over 100,000 cores. The library also supports mesh partitioning through interfaces to several packages, including Hilbert space filling curves [127] and graph-based algorithms [128]. In addition to external solver packages such as PETSc [129] and Trilinos [130], libMesh offers support for multiphysics applications through automatic assignment of variables to PETSc field splits and identification of subdomains within a mesh thus, enabling physics-aware algorithms and adaptive modeling algorithms. Recently, libMesh has extended its capabilities to include the f_parsere library for easy specification of boundary conditions, initial conditions, or constitutive equations from an input file.

5.3.3. Heat source modelling for SLM

Selective Laser Melting (SLM) is an additive manufacturing technique that uses a high-power laser beam to selectively melt and fuse metal powder particles, layer by layer, to form a 3D object. In SLM, the energy of the laser beam is typically absorbed by the metal powder particles, which then melt and solidify to form the object. However, the process can also generate heat, affecting the final product's microstructure and mechanical properties. One way to model the heat generated

in SLM is to use a volumetric heat source term in the heat transfer equation. The Double Ellipsoid Volumetric Source (DEVS) model is a commonly used approach to represent the heat source in SLM (see Figure 24). In this model, the laser beam is represented by two overlapping ellipsoids, each with its power density and orientation. The overlapping region between the two ellipsoids represents the hottest part of the laser beam, where the highest power density and temperature are reached. The DEVS model takes into account the size, shape, and orientation of the laser beam, as well as the absorption and scattering properties of the metal powder. It has been shown to provide accurate predictions of the temperature distribution and melt pool geometry in SLM and can be used to optimize process parameters such as laser power, scanning speed, and powder layer thickness.

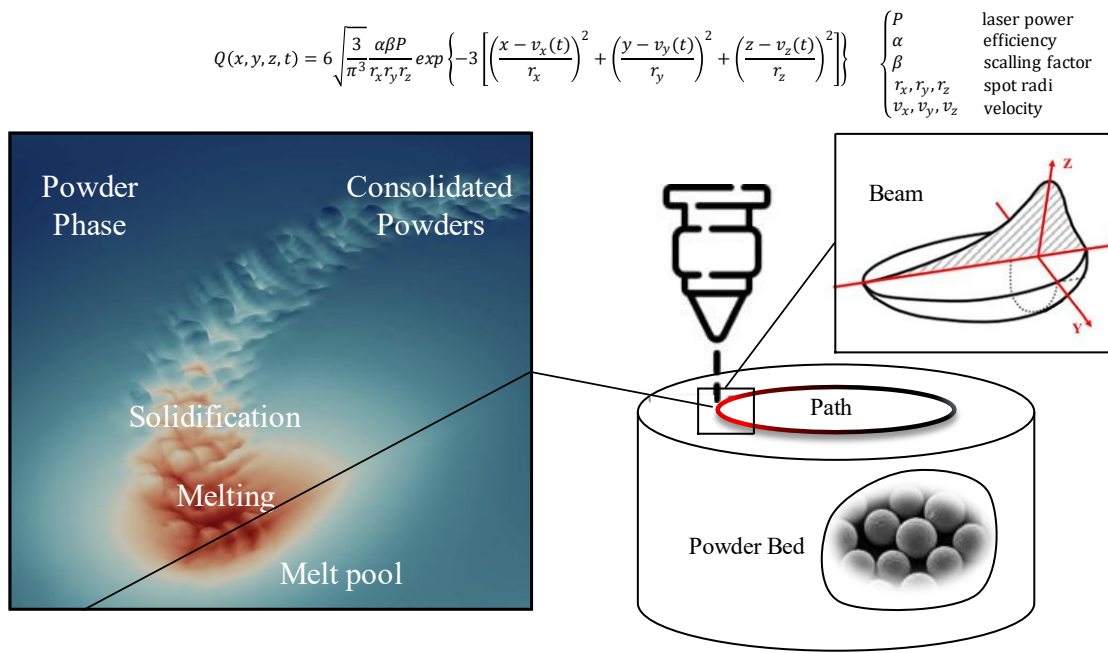


Figure 24 Schematic of Multiphysics phenomenon of PBF process.

5.4. Finite element method and implementations for thermomechanical phase field in AM processes

In order to address the objectives at hand, the problem of additive manufacturing will be tackled through a comprehensive numerical approach, employing the finite element method (FEM). This discussion will shed light on the crucial role played by material properties in the context of phase change and the resulting residual stresses. The proposed modeling approach, known as phase-field thermo-elasto-plasticity, involves three primary variables: temperature (T), phase-field (ϕ), and displacement (u). These variables collectively govern the behavior of the system and are fundamental to accurately capturing the underlying physics. First, the thermo-mechanical and

phase-field equations will be solved using two techniques: fully coupled and uncoupled. Both methods offer distinct advantages and present unique challenges. By considering both approaches, a comprehensive understanding of the system's behavior can be obtained. In the fully coupled technique, the thermo-mechanical and phase-field equations are solved simultaneously, taking into account the mutual interaction between temperature, phase-field, and displacement. This approach provides a more accurate representation of the complex interplay between these variables. However, it requires solving a highly coupled system of equations, which can be computationally demanding. Alternatively, the uncoupled technique decouples the thermo-mechanical and phase-field equations, solving them independently. This simplifies the computational process, but at the expense of neglecting the direct influence of one variable on the others. Despite its limitations, the uncoupled technique can still provide valuable insights into the system's behavior. Following the resolution of the thermo-mechanical and phase-field equations, the next step involves solving the precipitation equation, as outlined in subsection 4.9. This equation establishes the relationship between displacement, phase-field, and chemical composition. The temperature results obtained from the previous parts serve as input for this step.

5.4.1. Boundary conditions

For both uncoupled and coupled formulation the initial and boundary conditions (BCs) are represented in Table 1, under the assumption of $\Gamma_D \cup \Gamma_N = \partial\Omega$ and $\Gamma_D \cap \Gamma_N = \emptyset$, with Γ_D and Γ_N indicating the Dirichlet- and Neumann-type boundaries, respectively.

Table 1 Governing initial and boundary conditions

Dirichlet B.C. (Γ_D)	$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}^*(\mathbf{x}, t) \quad \text{on } \Gamma_{D_u},$ $\phi(\mathbf{x}, t) = \phi^*(\mathbf{x}, t) \quad \text{on } \Gamma_{D_\phi}$ $T(\mathbf{x}, t) = T^*(\mathbf{x}, t) \quad \text{on } \Gamma_{D_T}.$
Neumann B.C. (Γ_N)	$-\kappa \nabla T \cdot \mathbf{n} = \mathbf{q} \quad \text{on } \Gamma_{N_T},$ $\nabla \phi \cdot \mathbf{n} = \mathbf{0} \quad \text{on } \Gamma_{N_\phi},$ $\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}^* \quad \text{on } \Gamma_{N_u}.$
Initial conditions	$T = T_{ref} \quad \text{on } \Gamma_{N_T},$ $\phi = \bar{\phi} \quad \text{on } \Gamma_{N_\phi}$ $\mathbf{u} = \bar{\mathbf{u}} \quad \text{on } \Gamma_{N_u}.$

5.4.2. Strong form of constitutive equations

In the uncoupled formulation, equation 4.35 is explicitly solved, and then the temperature equation is coupled with the phase-field equation. Subsequently, the temperature and phase-field equations are further coupled with the body equilibrium equation. Therefore, in the decoupled form, we have two residual equations. In coupled problems, equation 4.31 is directly solved by

simultaneously considering the temperature and body equilibrium equations. This approach involves solving the temperature and body equilibrium equations together, resulting in three independent residual equations.

Table 2 Strong form equations governing the coupled problem

Momentum balance	$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$
Phase-field evolution for Allen-Cahn	$\dot{\phi} = -M \left[W g'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) - \text{div}(l^2 \nabla \phi) \right]$
Phase-field evolution for Wang et al.	$\dot{\phi} = -\frac{1}{6\sqrt{2}\delta L/\mu_\phi T_M^2} \left[\frac{1}{4\sqrt{2}\delta T_M/12\omega} g'(\phi) - \Phi(T) p'(\phi) - \text{div}(l^2 \nabla \phi) \right]$
Coupled temperature evolution	$c\dot{T} = D + T \frac{\partial(\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - D)}{\partial T} - \left[\rho L \left(\frac{T}{T_M} \right) p'(\phi) + W g'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) - \text{div}(l^2 \nabla \phi) \right] \dot{\phi} - \text{div} \mathbf{q} + Q$
Uncoupled temperature evolution	$c\dot{T} = -\text{div} \mathbf{q} + Q$

5.4.3. Weak forms of constitutive equations

The FEM can be utilized to implement the formulation outlined in the previous section by using the weak form of the governing PDEs given in Table 2. To accomplish this, arbitrary test functions associated with the field variables are employed and are multiplied by their respective PDEs, generating the weak forms as detailed below,

$$\mathbf{r}_u = \int_{\Omega} \boldsymbol{\sigma} \mathbf{B}_u^T dV - \int_{\Gamma_{N_u}} \mathbf{t}^* \mathbf{N}_u^T dS, \quad (5.2)$$

where $\mathbf{r}_u$, the residual vector associated with the displacement field. The residual form of the phase field equation for coupled method is presented as follows:

$$\begin{aligned}
\mathbf{r}_\phi = \int_{\Omega} & \left[\frac{1}{M} \dot{\phi} [N_\phi]^T N_\phi - 2W\phi(1-\phi)(1-2\phi)[N_\phi]^T \right. \\
& \left. - 30\Theta(T)\phi^2(1-\phi)^2[N_\phi]^T + l^2[B_\phi]^T[B_\phi] \right] dV \\
& - \int_{\Gamma_{N_\phi}} l^2 [B_\phi]^T [B_\phi] [N_\phi] dS,
\end{aligned} \tag{5.3}$$

The residual vector associated with the temperature field for two types of fully coupled method yields:

$$\begin{aligned}
\mathbf{r}_T = \int_{\Omega} & \left(c \dot{T} - \left[\rho L \left(\frac{T}{T_M} \right) p'(\phi) + W g'(\phi) + \rho L \left(\frac{T_M - T}{T_M} \right) p'(\phi) \right. \right. \\
& \left. \left. - \text{div}(l^2 \nabla \phi) \right] \right) [N_T] dV - \int_{\Gamma_{N_T}} \kappa [B_T]^T [N_T] dS \\
& + \int_{\Omega} \kappa [B_T]^T [B_T] dV + \int_{\Omega} Q [N_T]^T dV = 0.
\end{aligned} \tag{5.4}$$

For the uncoupled method associated with the decoupled phase field variable, the residual form is:

$$\begin{aligned}
\mathbf{r}_T = \int_{\Omega} & \dot{T} \frac{de}{dT} [N_T] dV + \int_{\Gamma_{N_T}} \kappa [B_T]^T [N_T] dS + \int_{\Omega} \kappa [B_T]^T [B_T] dV \\
& + \int_{\Omega} (\nabla \omega) \cdot (k \nabla T) d\Omega + \int_{\Omega} Q [N_T]^T dV = 0
\end{aligned} \tag{5.5}$$

$\frac{de}{dT}$ represents the heat capacity parameter is updated through equation (4.57) if the consolidation parameter, ψ is updated and through equation (4.57) if the consolidation parameter, ψ does not change.

$$\frac{de}{dT} = c_s(\psi) + \frac{dp(\psi)}{dT} \{L_0 + [c_l - c_s(\psi)](T - T_m)\} \tag{5.6}$$

$$\begin{aligned}
\frac{de}{dT} = \frac{dc_s(\psi)}{dT} T + c_s(\psi) + \frac{dp(\phi)}{dT} \{L_0 + [c_l - c_s(\psi)](T - T_m)\} \\
- p(\phi) \frac{dc_s(\psi)}{dT} (T - T_m)
\end{aligned} \tag{5.7}$$

In these equations, ϕ is solved with approximative temperature function as:

$$p(\phi) = (\phi)^3 \{10 - 15(\phi) + 6(\phi)^2\} \quad (5.8)$$

$$\phi = 0.5 \left\{ \tanh \left\{ A \left(\frac{T - T_m}{T_l - T_s} \right) \right\} + 1 \right\} \quad (5.9)$$

where A is a parameter controlling the steepness of the smooth phase change transition [131] and is here set to 5 as proposed in [24]. T_l, T_s are liquidous and solidus temperatures respectively.

5.4.4. ABAQUS Environment for uncoupled approach

ABAQUS is a well-known simulation tool used in additive manufacturing due to its advanced modeling capabilities for both thermal and mechanical phenomena. In this part of our study, we utilized ABAQUS to implement a thermal and mechanical uncoupled analysis for the DED process. That procedure allowed us to study the individual factors affecting the performance of the additively manufactured part without considering the interaction between thermal and mechanical behavior. By using ABAQUS for our simulations, we could accurately model the thermal behavior of the DED process, including the effects of heat transfer and phase changes, as well as the mechanical behavior of the resulting structure.

5.4.4.1. Thermal code execution

The heat transfer analogy described in Chapter 4 can be implemented in ABAQUS by utilizing the user thermal behavior of the material through the user subroutine UMATHT. This subroutine allows you to define the specific thermal behavior of the material within your ABAQUS simulation. Taking advantage of the heat transfer analogy allows for the implementation to be carried out at the integration point level using built-in temperature elements with DC3D8 (Hex-8 linear heat transfer). This approach leverages the capabilities of the in-built temperature elements in ABAQUS, allowing for more efficient and accurate simulations of heat transfer phenomena within the material. At the start point of the algorithm, the global variables declared in the UEXTERNALDB user subroutine can be initialized. A solution-dependent state variable (SDV) was allocated to the material state as powder phase at a time instant. When the powder phase changes by applying heat source via user DFLUX subroutine, the SDV changes to one and after cooling down this variable is fixed to one to be dedicated to fully solid material properties. Continuum-scale material adding is facilitated by the UEPACTIVATIONVOL subroutine, which interprets the event series information for material deposition caused by laser motion. This subroutine allows for the incorporation of material addition events at the continuum scale, enabling simulations that capture the deposition process accurately within the context of the larger material domain. The UMATHT subroutine reads the temperature at each material point at the end of each increment. Then it updates the consolidation value of those material calculation points which meet the state change criterion. The derivative of the internal energy concerning the

temperature resorting to the phase-field variables includes the enthalpy function to take into account of latent heat account by the fraction of different phases. In the end, a USDFLD subroutine is developed to manage the material states at the end of each time increment and store it. FILM and RADIATE subroutines are called to apply the heat boundary condition for convection and radiation, respectively. It is worth to be noted that, to overcome the issue of iteratively changing the convective and radiative boundary condition during the element activation, the load type labels, FFS and RFS, were used in ABAQUS to automatically define the thermal loads for the film coefficient and radiation only at the open faces of the elements after activation. Besides, COMMON blocks play critical roles in transferring information between all subroutines in detailed it has been shown in Figure 25.

Algorithm	Thermal Modelling
------------------	-------------------

```

procedure UEXTERNALDB
  if LOP=0 then
    Initialize the set of state variables at time  $t_0$ 
    Solid State :  $\varphi = 0$ 
    Powder Material :  $\psi = 0$ 
  end if
end procedure
procedure UEPACTIVATIONVOL
  Element activation for mass rate
end procedure
procedure DFLUX
  Apply the volumetric heat flux for laser heat source:
  
$$U(x, y, z, t) = \frac{fP}{\pi r_l^2} \exp(-f \frac{x^2 + (y-v)^2}{r_l^2})$$

end procedure
procedure UMATHT
  Transfer heat source by common block from DFLUX
  Update the state variables for  $\varphi$  and  $\psi$ 
  Set the material properties depends on temperature:
  
$$k(\psi) = (1 - \psi)k_p + \psi k_d$$


$$C_s(\psi) = (1 - \epsilon_0(1 - \psi))C_d$$

  Using the Galerkin weighted residual method to obtain the classical
  integral form to solve the non-linear thermal equations:
  Internal thermal energy (enthalpy) for unit of mass:  $e$ 
  Derivative of internal energy with respect to temperature:  $\frac{de}{dT}$ 
  Heat flux vector with respect to temperature:  $\hat{q} = -k(\psi)\nabla(T)$ 
  Variation of heat flux vector to temperature:  $\frac{\partial \hat{q}}{\partial T}$ 
  Variation of heat flux vector to the spacial gradient of temperature:
  
$$\frac{\partial \hat{q}}{\partial \frac{\partial T}{\partial x}} (i = 1, 2, 3)$$

end procedure
procedure USDFLD
  Transfer state variables by common block from UMATHT
  Store state variables and go to the next time increment
end procedure

```

Figure 25 User subroutines algorithm for the implementation of diffusive phase function model in phase changing exploiting the analogy with heat transfer.

5.4.4.2. Mechanical code execution

The above system of equations is implemented in ABAQUS by user coding in FORTRAN language and through a combination activation element regime with UEPACTIVATIONVOL subroutine and predefined temperature field from thermal analysis (as a load). UEXPAN user interface, as described in Figure 26, is embedded into the procedure to calculate the thermal strains. UMAT subroutine is called at all material points to perform constitutive model integration and returns updated stresses and the Jacobian. It is worth noting that the scenario was executed using in-built structural elements such as the C3D8 (Hex-8 linear brick element) type.

Algorithm	Mechanical Modelling
procedure	USDFLD
	Transfer state variables by common block from UMATHT
	Store state variables and go to the next time increment
end procedure	
procedure	UEPACTIVATIONVOL
	Element activation for mass rate
end procedure	
procedure	UEXPAN
	Calculate $\epsilon_{thermal} = a(T)_i T$
end procedure	
procedure	UMAT
	Solve $[K]du = dF$
	update $u = u + du$
	Recalculate strain and stress:
	$\epsilon = Bu$
	$\epsilon_{elastic} = \epsilon - \epsilon_{plastic} - \epsilon_{thermal}$
	$\sigma = E\epsilon_{elastic}$
	if $\sigma > \sigma_{Yield}$, then <i>correct</i>
	$\epsilon_{plastic}$, $\epsilon_{elastic}$, and σ
	Assemble nodal force $\{dF\}$
end procedure	

Figure 26 User subroutines algorithm for the implementation of thermo-elastoplastic material framework.

5.4.5. MOOSE Environment for fully coupled approach

The above FE system is implemented by resorting to the capabilities of the open-source software MOOSE. This software utilizes a collection of kernels that represent the physical phenomena being modeled. In every problem, these kernels assemble the governing PDEs' residuals at the element level and then pass the residuals to a global matrix. Subsequently, these residuals are used to update the solution via a nonlinear solver. All kernels can support automatic differentiation (AD) for residual calculations. In this study, we use the predefined Jacobian Free Newton Krylov (PJFNK) solver method, a variant of the Newton-Raphson method. The PJFNK utilizes a Krylov subspace technique to approximate the action of the Jacobian matrix on a given vector, rather than computing the Jacobian matrix explicitly, which can be significantly beneficial

in large-scale simulations or problems with complex physics, given that it is cost-effective to avoid the storage and computation of the Jacobian matrix. This method in MOOSE uses the preconditioned conjugate gradient (PCG) technique as the Krylov solver. Besides, to improve the numerical stability and precision of the nonlinear solutions, we used the MOOSE's automatic scaling feature which can bring different physics Jacobians as close to unity as possible.

5.4.6. Thermomechanical phase field chemical process of precipitation

A phase field method is a computational tool used to simulate complex systems with multiple phases and interfaces. To simulate a specific system, a set of PDEs is used to describe the evolution of different variables, and a free energy function is defined based on the underlying physics. To couple the phase field model with other physics such as mechanics or heat conduction, one can use the MOOSE-Phase Field module, which provides a range of tools to develop a phase field simulation with equations solved using FEM. The different phases in the simulation have separate free energies and may have varying mechanical and thermal properties. To accurately simulate the behavior of a system using the phase field method, the free energy of each individual phase must be determined. One possible approach to this involves using a “*Material*” object that encapsulates all necessary free energy derivatives and utilizes symbolic differentiation. The global free energy is then constructed by combining the free energies of each phase using non-conserved order parameters that indicate the distribution of the phases. Importantly, the derivatives of the phase-free energies are also used to construct the derivatives of the global free energy. Total free energy of the system which was presented in Equation 4.73 can be reformulated in MOOSE based on f_{local} , local energy term, f_{grad} , gradient energy term, f_{el} , elastic energy term respectively:

$$F = \int (f_{local} + f_{grad} + f_{el}) dV \quad (5.10)$$

Here, we used a the common approach of utilizing a linear combination of free energy densities f_{local}^j of every single phase in the system based on the provided model by Wheeler et al. in [132]. The local energy term combines the interfacial and chemical free energy terms (Equations 4.74 and 3.75) for every single phase like:

$$f_{local} = \sum_j h(\eta_j) f_{local}^j(\chi_{Al}, \chi_{Nb}) + Wg(\eta_j) \quad (5.11)$$

$h(\eta_j)$ is the switching function which varies smoothly from 0 to 1 as η_j goes from 0 to 1. Along two-phase interfaces, the switching function can be represented as: $h(\eta_j) = \eta_j^3(10 - 15\eta_j + 6\eta_j^2)$.

The barrier function is $g(\eta_j)$, which is multiplied by barrier height W , is often used in the context of phase transitions and is a measure of the degree of mixing of different phases in a system. The barrier function, W is defined as the difference between the actual composition of the system and the composition of the nearest pure phase region. Thus, the barrier function $g(\eta_j) = \eta_j^2(1 - \eta_j)^2$ multiplied by the barrier height W penalizes phase mixtures over pure phase regions. This penalty “encourages” the system to minimize the degree of mixing and to form pure phase regions, which is often the thermodynamically preferred state. On the other hand, the sum of the weights of all phases present at any given point in the simulation volume must be equal to 1 (i.e., $\sum \eta_j = 1$). This ensures that the system is in equilibrium and that the total free energy of the system is minimized. If this constraint is violated, the system will not be in equilibrium and will tend to evolve towards a new equilibrium state where the constraint is satisfied. The principle behind this constraint is known as the phase rule or Gibbs’s phase rule, which governs the behavior of multi-phase systems in thermodynamics.

$$k(\eta_j) = \sum_j h(\eta_j) - 1 = 0 \quad (5.12)$$

It should be noted that this constraint cannot spontaneously be satisfied and needs to be enforced. In MOOSE, we used the Lagrange multiplier technique to enforce the sum of all phase contributions to be one at every point in the simulation cell. A Lagrange multiplier λ should then be added to the Allen-Cahn equation as a field variable. The variational statement of the computational domain is then defined as: (η_j, λ) such that the following boundary conditions are satisfied:

$$a_j(\eta_j, v) + \int_{\Omega} \lambda \frac{\partial k}{\partial \eta_j} v \, dx = 0 \quad (5.13)$$

$$\int_{\Omega} q \frac{\partial \lambda k}{\partial \lambda} \, dx = 0 \quad (5.14)$$

The represented equations hold for all admissible test functions (v, q) and $a_j(\eta_j, v)$ is a weak form of Allen-Cahn equation(s). It is worth to be noted that we need a modified constraint condition (Equation 5.15)

$$k(\eta_j, \lambda) \equiv k(\eta_j) - \frac{\varepsilon}{2} \lambda \quad (5.15)$$

due to the complexity of Equation 5.15 in preconditioning and iteratively solving the system of equations. The additional term of $\frac{\varepsilon}{2} \lambda$ represents the $\mathcal{O}(\varepsilon)$ which is a function of λ and dependent to the constraint condition. This condition leads to a non-zero value on-diagonal Jacobian

contribution of ε for Equation 5.15, avoiding “zero pivot” errors arising from **PTESc** preconditioners, e.g. **-pc_type lu**, that implements only partial pivoting. The value ε should be selected by trading off between accuracy and solver performance. This approach violates the $\mathcal{O}(\varepsilon)$ constraint, which requires the error to be proportional to ε . However, it has been discovered that this deviation does not have a negative impact on the overall quality of the solution, and it actually enhances the convergence characteristics of the solver. Moreover, we used Voight-Taylor scheme [133] in MOOSE platform including the elastic constants, constitutive model (stress), and eigenstrain, which can depend on composition variables. The proposed simulation algorithm is equipped with an adaptive time step, which is automatically adjusted based on the rate of evolution of the phase field variables. The computational time required for a phase field simulation depends on several factors, including the total time of the thermal history and the complexity of the simulation process, such as the presence of nucleation, precipitate growth, or the absence of precipitates. In this fully implicit manner, the maximum time step allowed in the simulation is also determined by the stability of the system. This means that the time step must be small enough to capture the relevant physical phenomena, but not so small that it unnecessarily increases the computational cost. This approach allows for the simulation to use larger time steps when the system is less active and smaller time steps when the system is undergoing rapid changes. All simulations are performed on a computer cluster equipped with 2 Intel CPUs (16 cores total), and 128 GB of RAM. The CPU nodes are connected via a 40 Gbps InfiniBand network, which allows for efficient communication between the CPU nodes and enables the efficient use of parallel computing resources.

5.4.6.1. Nondimensionalization of phase field parameters

The phase field model needs to use non-dimensionalized parameters for optimizing solution purposes. The process of nondimensionalization involves defining characteristic scale values for the length, energy, and time of a system and using these values to normalize the equations. By doing so, the resulting equations become dimensionless, and the physical quantities are expressed as ratios of their respective characteristic scale values. The length scale is governing by Allen Cahn formulation (Equation 4.89), herein is $l_0 = 0.5$ (nm). All energy terms are normalized by $E_{Norm} = 1.49 \times 10^8$ (J/mol) and mobility terms are normalized with $M_{Norm} = 2.42 \times 10^{-19}$ (mol²/Nsm²). The time (t) is divided by the diffusion timescale, resulting in a nondimensional time variable (t^*), defined as $t^* = t D_{Nb} / (l_0^2)$. This transformation scales the time variable such that it is in units of diffusive time, making it more convenient for numerical simulations.

5.4.6.2. Nucleation with the stochastic tools

In the case of the isothermal process in the presence of the almost constant temperature, the nucleation events occur simultaneously, which means that multiple nucleation sites are formed and then may disappear at the same time. The specific conditions that lead to homogeneous nucleation at this temperature and for this material (Ni-Nb-Al) may be influenced by factors such as composition, crystal structure, and cooling rate. In MOOSE environment, the temperature effects can be replaced by Langevin noise [134] in simulations of nucleation by introducing random fluctuations that mimic the thermal fluctuations of the system being studied. Those random fluctuations can be added to the chemical potential term resorting to a stochastic differential equation that includes a random noise term. The amplitude of the noise term can be adjusted to match the expected level of thermal fluctuations at a given temperature. By adding the noise term $\xi(t, \vec{r})$, to the Cahn-Hilliard equations as: $\partial\chi/\partial t = \dots + \xi(t, \vec{r})$. Those random fluctuations can be added to the chemical potential term by resorting to a stochastic differential equation that includes a random noise term. The amplitude of the noise term can be adjusted to match the expected level of thermal fluctuations at a given temperature. By incorporating the noise term $\xi(t, \vec{r})$ into the Cahn-Hilliard equations as follows: $\partial\chi/\partial t = \dots + \xi(t, \vec{r})$. In finite element solutions, the residual and Jacobian terms are typically recomputed multiple times per step. To ensure that the noise field is consistent throughout the time step, the same random seed must be used for all calculations during that time step. This ensures that the same noise field is used in all parallel processes, regardless of the number of processors used for the simulation [135]. On the other hand, during laser processing, such as in additive manufacturing or laser surface treatment, the local temperature of the material can rapidly increase and cause the formation of nuclei, which are small clusters of atoms or molecules. The nuclei can then grow into larger particles through the process of nucleation and precipitation. However, if the nuclei do not reach a critical size, they may dissolve back into the material before they have a chance to grow. It is common to use probability functions in nucleation simulations to determine the likelihood of nucleation events occurring at a given time and temperature (see Figure 27). These probability functions are typically based on classical nucleation theory (CNT) and are used to model the rate of nucleation as a function of the relevant thermodynamic parameters. MOOSE has a “*DiscreteNucleationInserter*” to generate a spatial smoothed map of all nucleation sites according to the nucleation rate, the critical nucleus size (herein, critical nucleus volume), and the nucleation site distribution function.

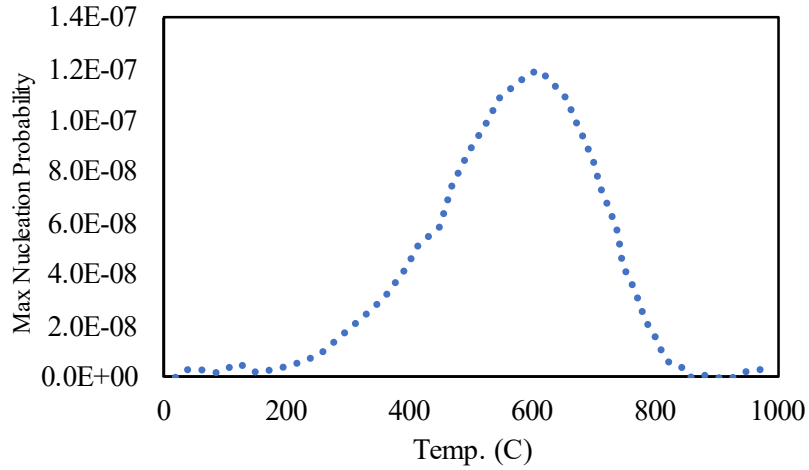


Figure 27 Nucleation probabilities as a function of temperature[136].

5.4.6.3. Thermodynamic database (TDB) CALPHAD

The CALPHAD approach is widely used for the evaluation and compilation of the thermodynamic and kinetic input data in quantitative PF modeling of multi-physics systems. Direct incorporation of the CALPHAD library into the MOOSE environment enables seamless access to extensive thermodynamic and kinetic databases, improving the accuracy and reliability of PF simulations [137].

5.4.6.4. Periodic boundary conditions (PBC)

Periodic boundary conditions (PBC) are a common technique used in numerical simulations to represent systems with periodicity in the systems with conserved quantities. PBC enforce value constraints on separate boundaries in the mesh by wrapping the boundaries of the simulation box such that they "connect" with each other, effectively creating a virtual periodic system [138]. This means that a particle that leaves the box from one boundary will re-enter the box from the opposite boundary, as if the simulation was performed in an infinitely repeating system. This technique is useful for modeling quasi-infinite domains, as it allows for a larger simulation box to be used without significantly increasing the computational cost. It is also useful for systems with conserved quantities, such as the total energy or momentum, where PBC can help to prevent any accumulation of errors over time due to numerical imprecisions or boundary effects.

5.4.6.5. Summary of the weak form of governing equations

The coupled interfacial, chemical and elastic energy terms in the free energy function include the PDEs for the various variables. In MOOSE, the FEM is utilized to implement the formulation outlined in the previous sections by using the weak form of the governing PDEs. The residual

form of equations for Allen-Cahn and Cahn-Hilliard (including two terms) and constitutive body equilibrium are presented in Equations 5.16 to 5.19. It should be noted that solving the Cahn-Hilliard equation with FEM is demanding, due to the existent of a fourth order gradient [139]. Herein, we used the approach of splitting the fourth order differential equation into two second order differential equations, using two separate variables, the concentration χ_i and the chemical potential μ_i , which are represented in equations 5.16 and 5.19.

$$\begin{aligned} \mathcal{R}_i(\eta_i) = & \left(\psi_m, \frac{\partial \eta_j}{\partial t} \right) + (\nabla(\kappa_j \eta_j), \nabla(L\psi_m)) + L \left(\frac{\partial f_{\text{local}}}{\partial \eta_j} + \frac{\partial f_{\text{ela}}}{\partial \eta_j}, \psi_m \right) \\ & - \langle L\kappa_j \nabla \eta_j \cdot \vec{\eta}, \psi_m \rangle, \end{aligned} \quad (5.16)$$

$$\mathcal{R}_i(\mu_i) = \left(\psi_m, \frac{\partial \chi_i}{\partial t} \right) + (M_i \nabla \mu_i, \nabla \psi_m) - \langle M_i \nabla \mu_i \cdot \vec{\eta}, \psi_m \rangle, \quad (5.17)$$

$$\mathcal{R}_i(\chi_i) = (\nabla \chi_i, \nabla(\kappa_i \psi_m)) - \langle \nabla \chi_i \cdot \vec{\eta}, \kappa_i \psi_m \rangle + \left(\left(\frac{\partial f_{\text{local}}}{\partial \chi_i} + \frac{\partial f_{\text{ela}}}{\partial \chi_i} - \mu_i \right) \psi_m \right), \quad (5.18)$$

$$\mathcal{R}_i(u_j) = (\psi_m, -\varrho). \quad (5.19)$$

Chapter 6

Models' Evaluation: Numerical and Experimental Examples

6.1.Introduction

In this section, numerical models are adopted to investigate the behavior of Inconel 625 at various computational scales. Building upon the previous discussion, the first subsection focuses on the uncoupled computational stage for the Directed Energy Deposition (DED) process. Material properties, which are temperature-dependent, and phase transitions are considered. The primary objective in single-track investigations is to analyze the temperature and morphology of the melt pool, as well as the resulting residual stresses and strains. Utilizing high-fidelity discretization techniques at the mesoscale, a lumped computational model incorporating thermal and mechanical aspects is developed for the multi-layer deposition process. At the macro-scale, the model emphasizes the effects of re-melting, re-solidification, and their impact on residual stresses and strains. Furthermore, the investigation explores the influence of thermal loads on the stability of thin-walled structures during the build process. Subsequently, significant findings regarding a fully coupled thermo-mechanical phase-field model for the Selective Laser Melting (SLM) process using the same material are discussed. The study aims to understand the reciprocal interactions between changing parameters and the corresponding responses in other fields.

6.1.Uncoupled PF model responses

6.1.1. Phase-Field parameters considerations

In the uncoupled formulation presented in section 4.5.2, we utilize a hyperbolic tangent function as an approximation for the formulation of equation 4.32. This approximation is derived from explicitly solving this equation, taking into account the behavior of the phase transition (Figure 28). By embedding the phase variable in equation 4.46, we incorporate the phase function approximation as Equation 6.1. This approach allows us to model the melting and solidification processes more efficiently and accurately, capturing the essential characteristics of the phase transition.

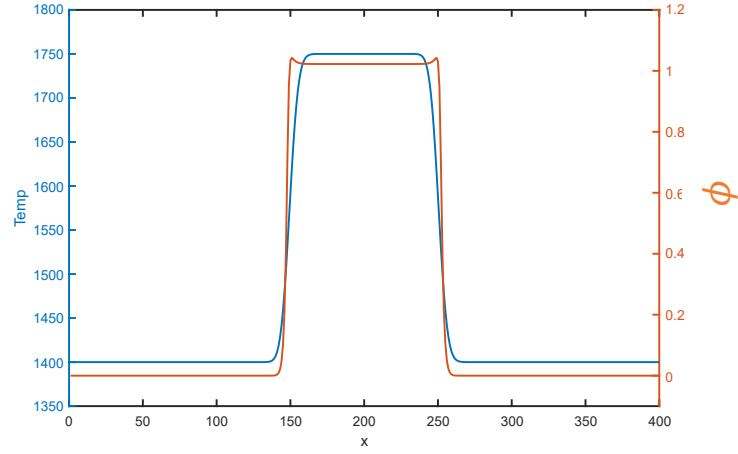
$$\phi = \frac{1}{2} \left\{ \tanh \left(A \frac{T - T_M}{T_L - T_S} \right) + 1 \right\} \quad (6.1)$$

in which A is a steep coefficient and T_M , T_L and T_S are melting, liquidous and solidus temperatures respectively. For both Wang and Allen-Cahn phase field models the PF parameters for Inconel 625 are presented in Table 3.

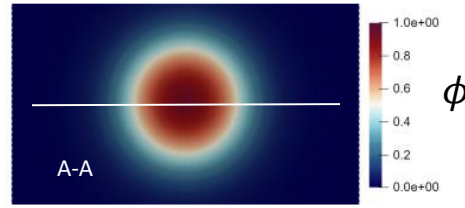
Table 3 Phase field parameters for Inconel 625 [140–142].

Parameters	Value	Units
Kinetic coefficient (μ_ϕ)	0.5	$mm \ K^{-1} s^{-1}$
Interface width (δ)	1	mm

Surface tension (ω)	65×10^{-6}	$mJ\ mm^{-2}$
Latent heat (L)	23.8×10^9	$mJ\ .tonne^{-2}$
Melting temperature (T_M)	1730	K



(a)



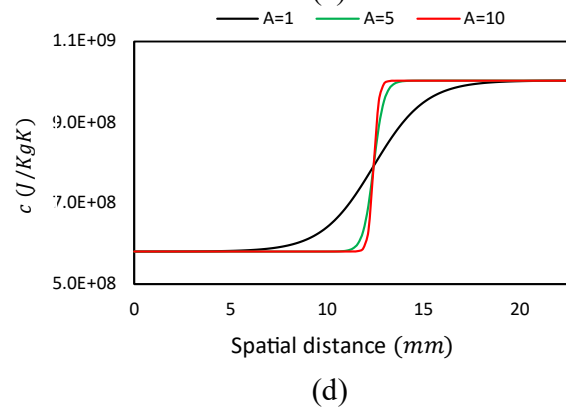
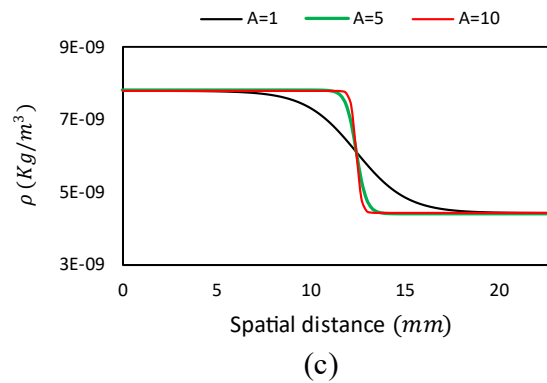
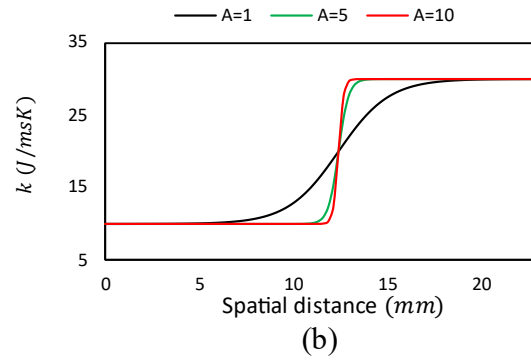
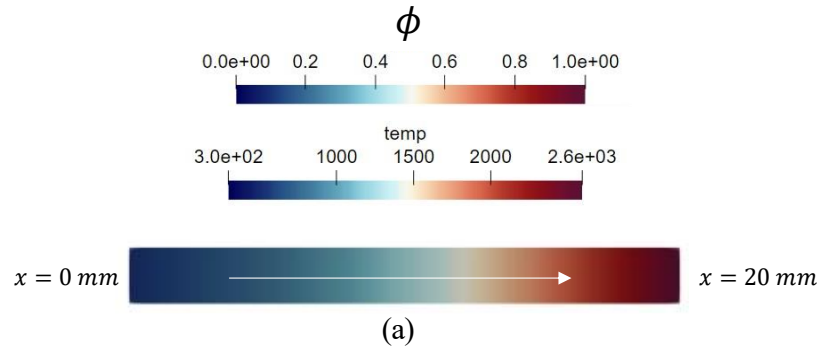
(b)

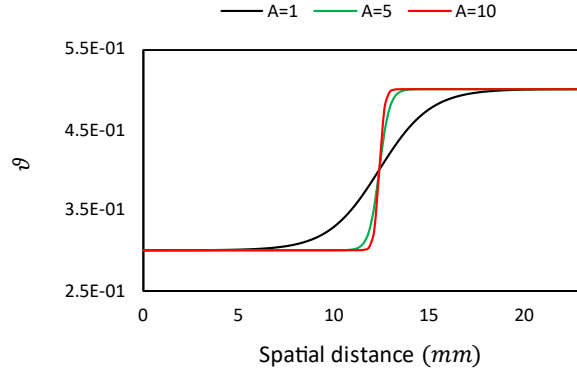
Figure 28 (a): Graph of the explicitly solved approximated phase field along A-A as it varies with temperature, (b): Phase field variable in the presence of a laser heat source.

Temperature unit in vertical axis is kelvin and spatial discretization in horizontal axis is μm .

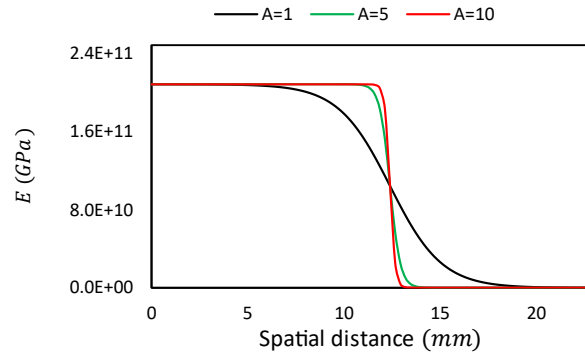
6.1.2. Temperature and phase-field dependent material properties

In the numerical simulation of the AM process using the FEM, the choice of the material properties and their dependencies on the temperature or the material state plays a vital role in the thermal and mechanical analysis [143]. For the transient temperature field computation, the material density (ρ), the thermal conductivity (k), and the heat capacity (c) are of particular importance. The Young's modulus (E), the yield stress (σ_y), the Poisson's ratio (ν), and thermal expansion coefficient (α) play a major role in the calculation of elastoplastic deformations and, thus, the residual stresses. In Figure 29 (a-g), material properties for an arbitrary domain in a temperature interval between solidus, $T_s = 1563\ K$, and liquid temperatures, $T_l = 1723\ K$, are depicted to shed light on the application of the phase field method in the tracking interfaces for material properties attribution due to the effect of the moving heat source.

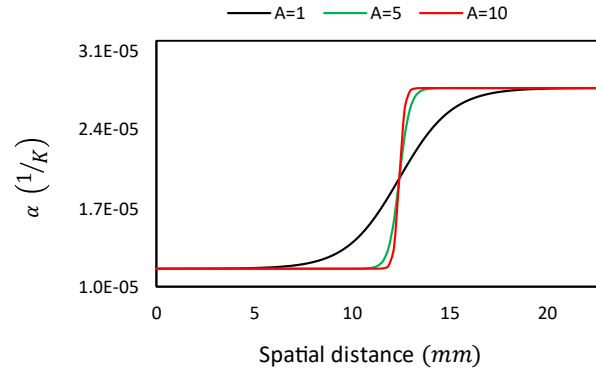




(e)



(f)



(g)

Figure 29 (a-g) Temperature and phase-field contours with various and phase-field-dependent derived material properties.

6.1.3. Single-track scale

For model calibration, a limited number of cladding lines from Inconel 625 powder were printed by various laser power, scanning speeds, and feed rates to investigate the model's capability in predicting the melt pool morphology. A tempered steel (42CrMo4) plate with size of $100\text{mm} \times 120\text{mm} \times 15\text{mm}$ was used as a substrate. The surface was machined and then cleaned by ethanol during the preparation process. The powder used is commercially the gas-atomized Nickel-based super alloy (MetcoClad 625), similar to Inconel 625. Figure 30 shows the micrography of the powder. Laser cladding experiments were performed by a coaxial laser

machine “LDF 3000 – 100” with a fiber-coupled high power laser diode (adjustable wavelength 900-1030 nm that changes depending on power), with 6000 W maximum beam power output. The laser machine was equipped with a 6-axes KUKA KR90 R3100 industrial robot. Based on Table 4, 18 different single tracks, 15 mm in length, were produced by altering three process parameters, namely laser powers P (1, 1.5, 2, 2.5, 3 kW), scanning speeds v (2, 4, 6, 10 mm/s) and powder feed rates F (10, 15, 20 gr/min). All other parameters remained constant throughout the experiments. The laser spot diameter was 2.5 mm with a top-hat beam profile. A high-purity argon (99.99%) as the shield gas, with a flow rate equal to 5.5 L/min, was utilized to minimize contamination and oxidization. The single tracks were cross-sectioned, mounted in resin and polished down to 1 μm diamond suspension as a last stage. The geometry measurements of height, depth and width of the cladding lines produced by the DED technique were achieved using a Leica DVM6 A 2019 digital microscope. Figure 31 (a-f) shows the geometrical measures of the clad section of the molten pool for some samples using the software ImageJ. Table 4 presents the measured value from designed experiments for Inconel 625 single tracks clad on 42CrMo4 entirely.

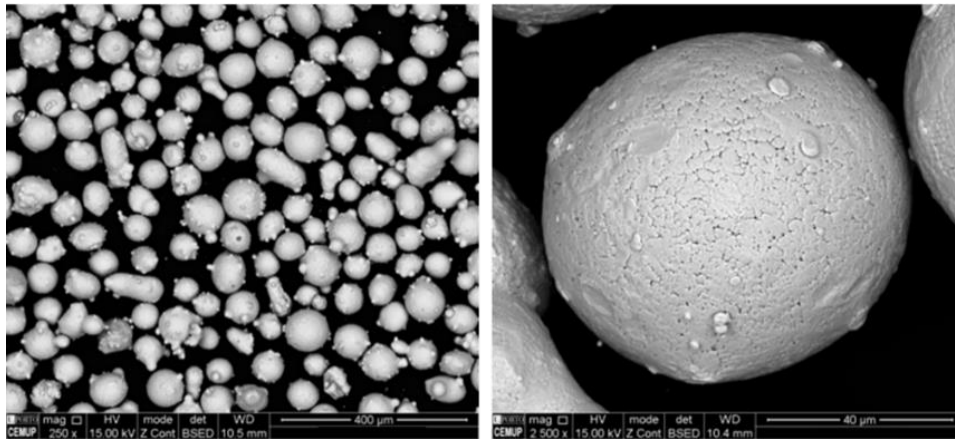


Figure 30 SEM micrograph of MetcoClad 625 powder.

Table 4 Measured value sets for width, height and penetration depth in single clads Inconel 625 on 42CrMo4 substrate.

Set No.	1	2	3	4	5	6	7	8	9
P-V-F	1_2_15	1_6_15	1.5_10_10	1.5_10_15	2_2_15	2_4_15	2_6_10	2_6_15	2_6_20
w (mm)	2.79	3.07	3.09	3.11	3.62	3.5	3.38	3.61	3.63
h (mm)	3.07	1.22	0.71	1.03	3.66	2.47	1.39	1.47	1.71
d (mm)	0.25	0.06	0.43	0.23	1.28	1.12	1.16	0.51	0.56
Set No.	10	11	12	13	14	15	16	17	18
P-V-F	2_10_10	2_10_15	2.5_10_10	2.5_10_15	3_2_15	3_4_15	3_6_10	3_6_15	3_6_20
w (mm)	3.2	3.36	3.33	3.46	5.05	4.64	3.89	4.71	3.94
h (mm)	1.2	0.81	0.86	1.23	3.4	2.06	1.85	0.78	1.55
d (mm)	0.72	0.88	1.04	1	2.06	0.89	1.08	0.68	1.34

The specific energy E and powder density D are calculated via Equations 6.2 and 6.3, where P, D_l, v and F are the laser power, the laser diameter, the scanning speed and the scanning feed rate respectively.

$$E(kW/mm^2) = P / D_l * v \quad (6.2)$$

$$D(gr/mm^2) = F / D_l * v \quad (6.3)$$

Then, the synergistic interaction between regression-based specific energy and powder density can be represented by Equations 6.4 and 6.5. The adjusted R-square values are 86.55% and 75.07% respectively for H (height of cladding layer) and W (width of cladding layer).

$$H(mm) = 0.51761 + 0.00025 E + 0.01083 D \quad (6.4)$$

$$W(mm) = 3.12365 + 0.00127 E - 0.00654 D \quad (6.5)$$

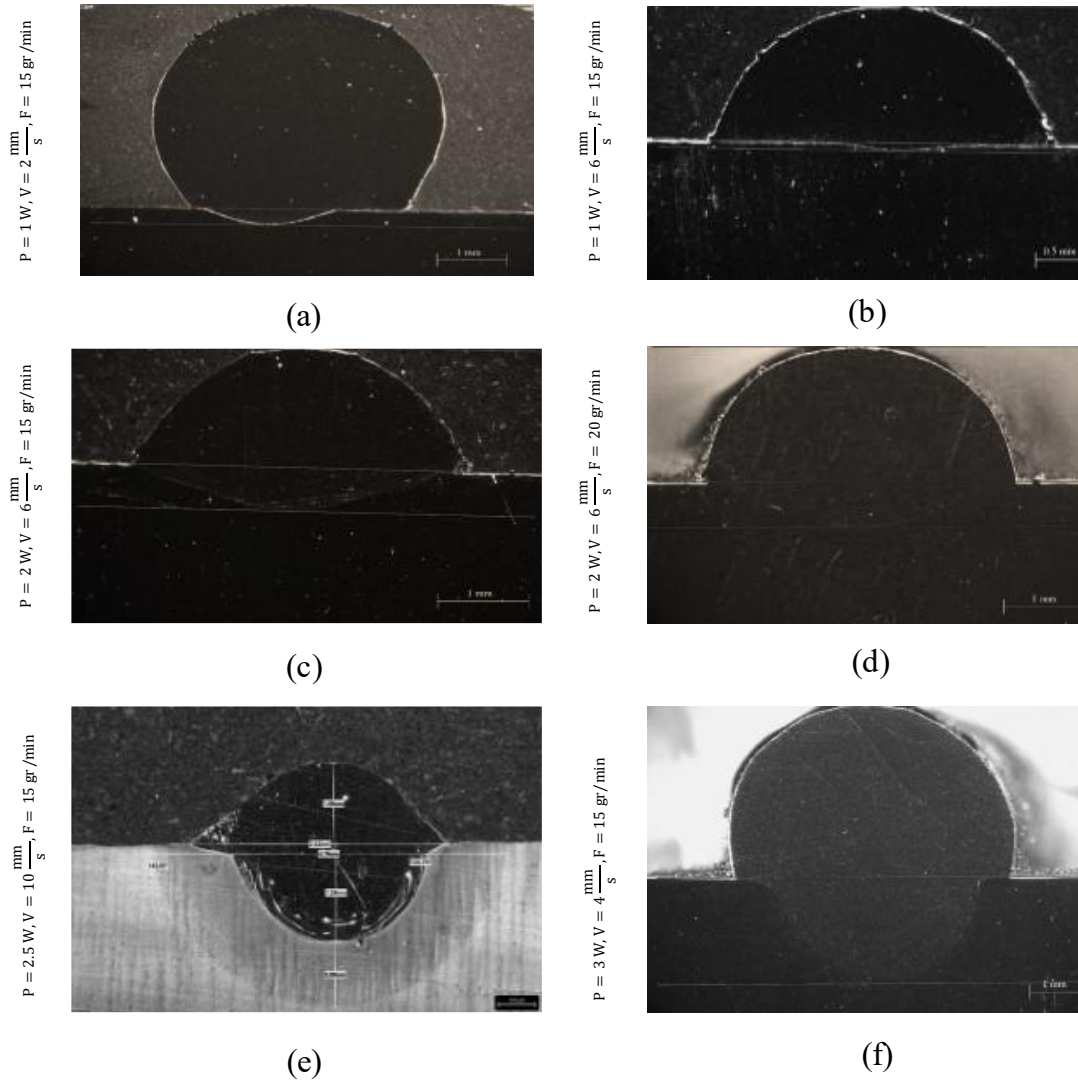


Figure 31 (a-f) selection of the cross sections of Inconel 625 single tracks cladded on 42CrMo4 substrate.

6.1.3.1. Transient heat model associated with phase field approach

Figure 32 (a,b) shows how the computed material state variables work with time and temperature; the red and blue regions denote the liquid phase and solid phase respectively and the region between them represents the mushy area.

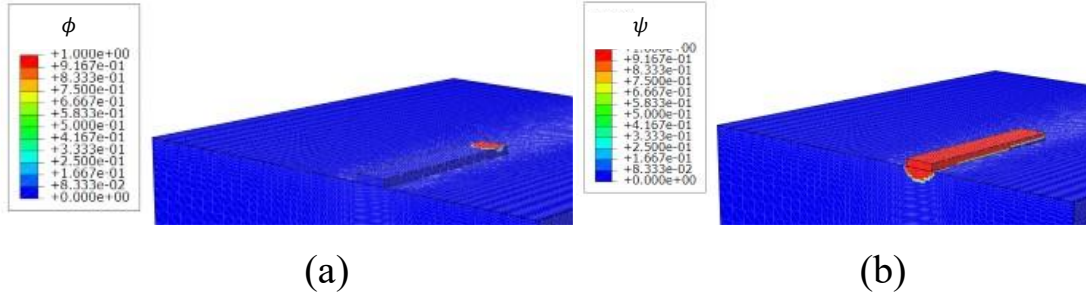


Figure 32 Material state variables represent (a): phase parameter ϕ , (b): consolidation parameter ψ
All for $P = 2 \text{ kW}$, $v = 10 \text{ mm/s}$, $F = 10 \text{ gr/min}$.

The presented graphs in Figure 33 (a-c) show the obtained results from the proposed model with a phase-field approach for various laser power values from 1.5 kW to 2.5 kW. The results indicate that increasing the laser power remarkably increases the temperature value and even material vaporization occurs. For two laser powers 2kW and 2.5kW vaporization is reached. As mentioned previously, the material phase variables include: ϕ_f , with red dotted lines, which represents the time of material changes from liquid to the solid phase, the parameter ϕ_v with purple dotted line which represents a time period of vaporization phase existence, and lastly, the dedicated parameter ψ (black solid line) for tracking consolidation, between powder and melt states. Before laser reaches and starts melting $\psi, \phi_f = 0$, after melting the temperature rises and material state variable ϕ_f changes to 1 which means the material state is liquid.

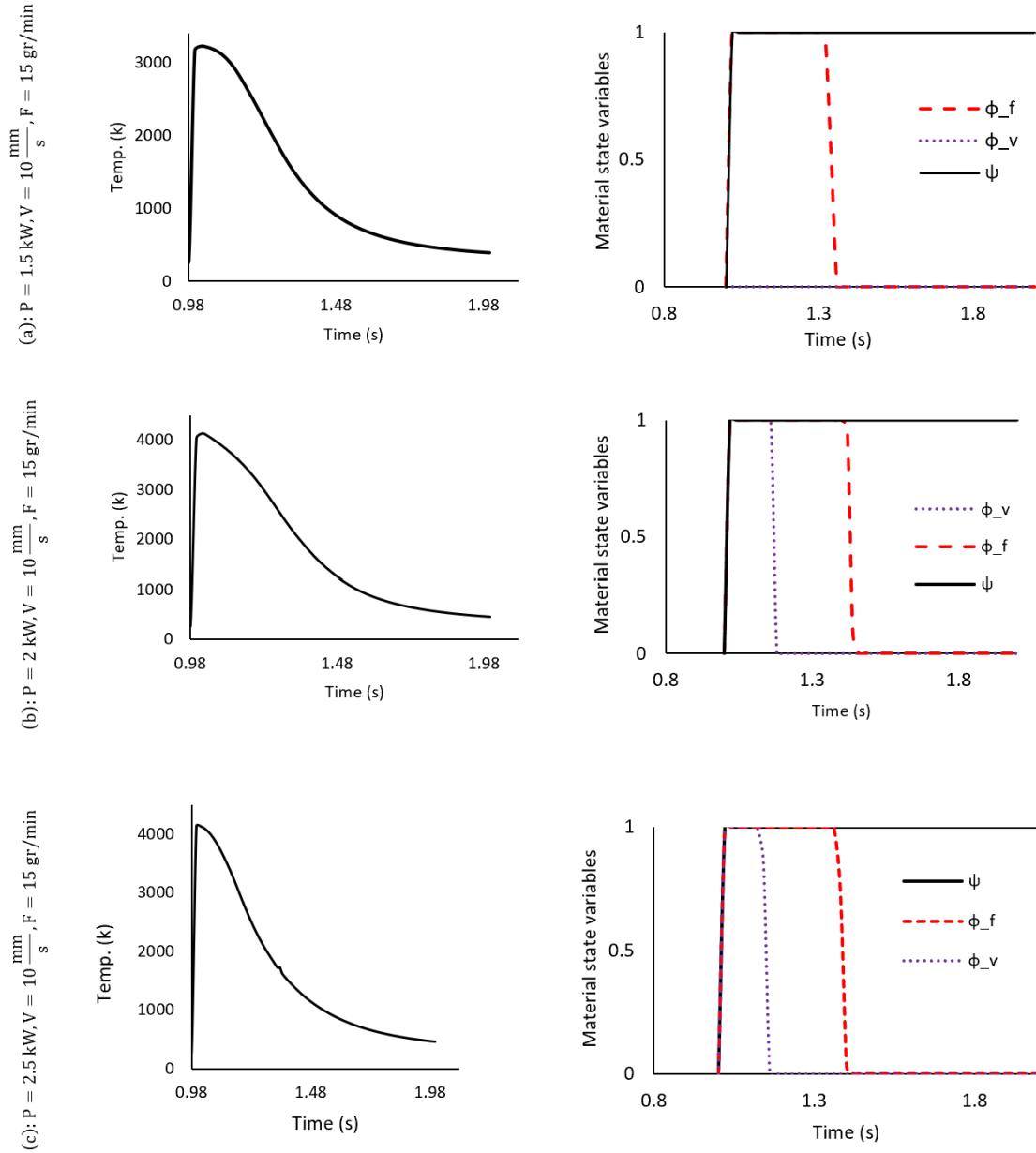


Figure 33 Temperature profile and material state variables with $SS = 10 \text{ mm/s}$, $FR = 15 \text{ gr/min}$ (a) $P = 1.5 \text{ kW}$, (b) $P = 2 \text{ kW}$, (c) $P = 2.5 \text{ kW}$.

Melt pool lifetime refers to the period time the liquid phase is present. The melt pool lifetime can be observed in Figure 34 for three different laser power values, an important parameter that determines the stability of the track formation during the process [144]. This graph illustrates that when the scanning speed and feed rate are fixed and the laser power increases, the melt-pool lifetime increases. The reason is that liquid phase lifetime depends not only on the scanning speed but also on the heat supply and volume of the melt pool. The liquid phase lifetime for laser power 1.5 kW is 54 ms and increases to 64 ms with laser power 2.5 kW .

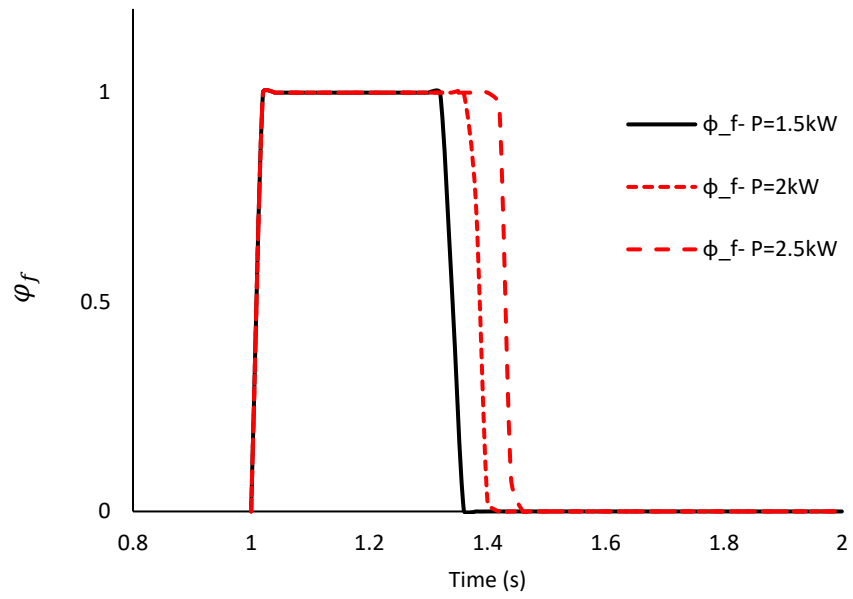


Figure 34 Liquid phase life-time comparison for changing laser powers from 1.5kW to 2.5kW versus time with the fixed scanning speed $SS = 10 \text{ mm/s}$ and feed rate $FR = 15 \text{ gr/min}$.

From Figure 35, the different lifetimes of the melt pool, by varying the scanning speed while the laser power and feed rate keep fixed, can be obtained. The results indicate that the melt pool lifetime tends to decrease gradually as the speed increase from 30 ms to 92 ms for 15 mm/s and 5 mm/s respectively.

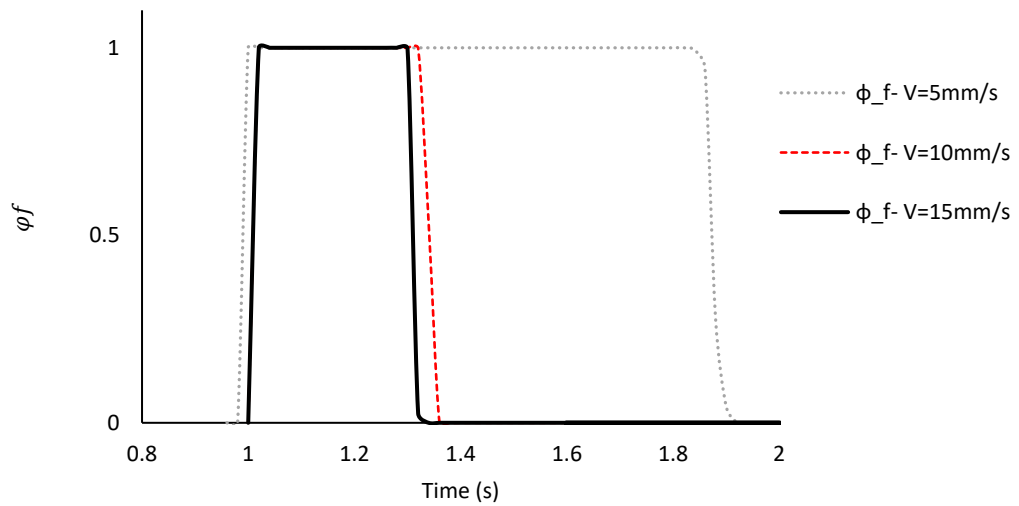


Figure 35 Liquid phase life-time comparison for changing laser scanning speed from 5 mm/s to 15 mm/s versus time with the fixed laser power $P = 1.5 \text{ kW}$ and feed rate $FR = 15 \text{ gr/min}$.

The results in Figure 36 (a-d) show the comparison between the experimental, from Table 4, and the obtained results from FEM simulations for the dimension of melt pools, including the height, width, and depth values. The proposed model can predict the melt pool dimension with reasonable accuracy. In Table 5, detailed information from Figure 34 (a-d) is provided for the same process parameters.

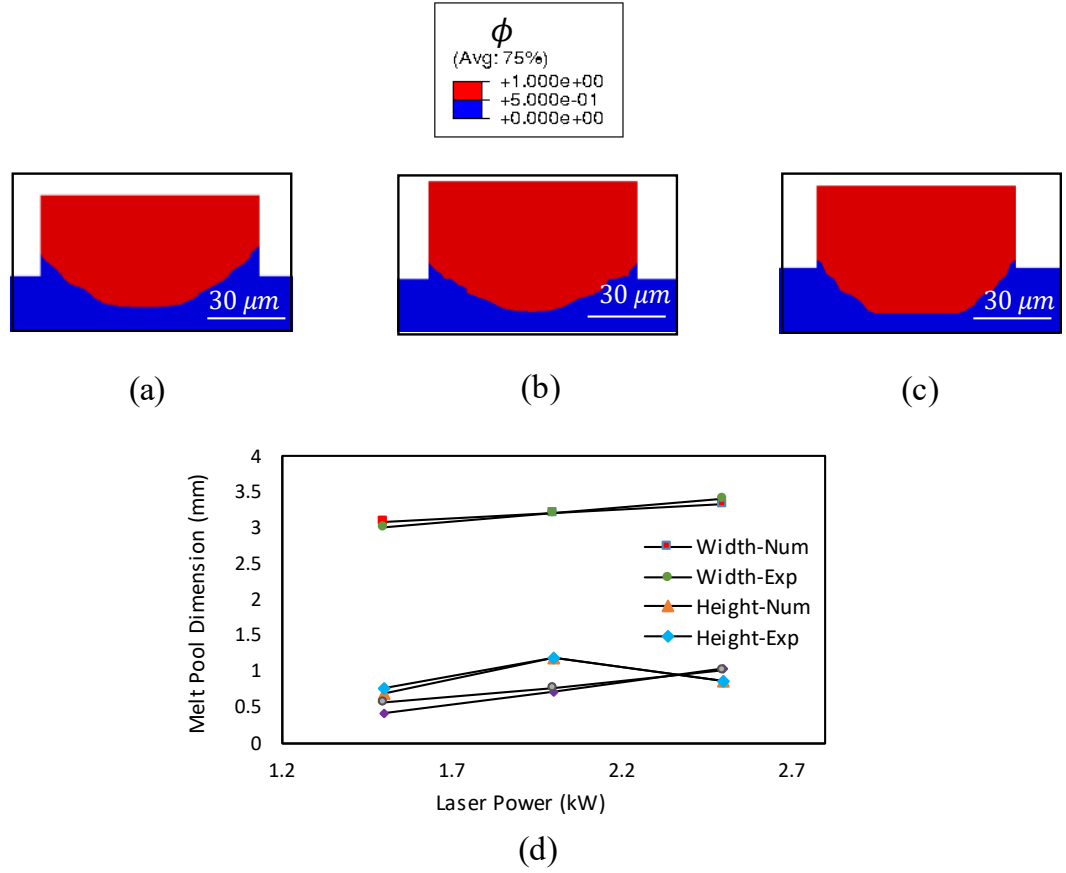


Figure 36 Predicted melt pool morphology in Z direction for single-track with $v = 10 \text{ mm/s}$, $F = 10 \text{ gr/min}$ (a): $P = 1.5 \text{ kW}$, (b): $P = 2 \text{ kW}$, (c): $P = 2.5 \text{ kW}$, (d): comparison of the predicted melt pool width with the experimental results from [24].

Table 5 Comparison of the melt pool size between experimental with numerical

Process Parameters	Width (Exp.)	Width (Num.)	Depth (Exp.)	Depth (Num.)	Height (Exp.)	Height (Num.)
$P = 1.5 \text{ kW}, v = 10 \frac{\text{mm}}{\text{s}}, F = 15 \text{ gr/min}$	3.11 mm	2.41 mm	0.23 mm	0.35 mm	1.03 mm	1.10
$P = 2.0 \text{ kW}, v = 10 \frac{\text{mm}}{\text{s}}, F = 15 \text{ gr/min}$	3.36 mm	3.25 mm	0.88 mm	0.85 mm	0.81 mm	0.8
$P = 2.5 \text{ kW}, v = 10 \frac{\text{mm}}{\text{s}}, F = 15 \text{ gr/min}$	3.46 mm	3.26 mm	1 mm	0.814 mm	1.23 mm	1.14

The red triangles and purple squares in Figure 37 show the average widths and depths of the simulated melt tracks at different scanning speeds. Figure 38 provides evidence that increasing the laser velocity decreases the volume of the melt pool. When the scanning speed is low, the laser remains longer around a local point, thereby generating more heat and resulting in a larger melt volume.

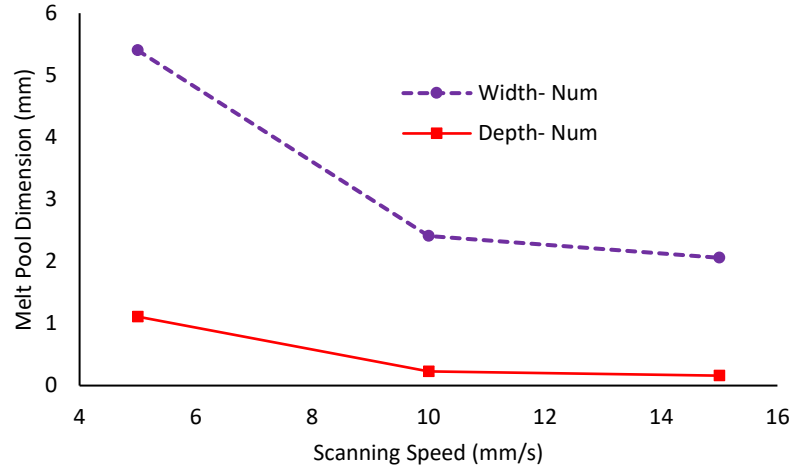


Figure 37 Predicted melt pool dimensions numerically for single-track scan with the fixed laser power $P = 1.5 \text{ kW}$ and feed rate $FR = 15 \text{ gr/min}$ and varying the scan speed.

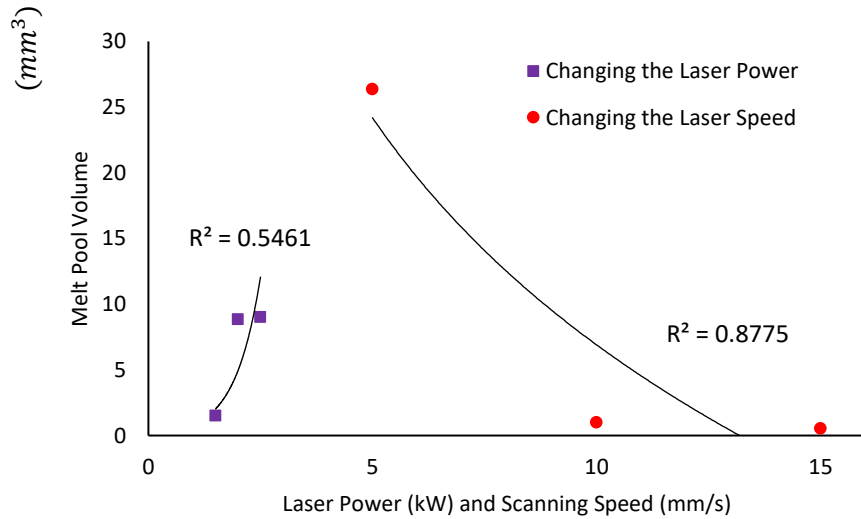


Figure 38 Melt pool volume in DED with different scanning speeds and powers.

6.1.3.2. Thermal Stability Analysis

The dynamics of transient heat transfer are commonly obtained via numerical time integration schemes such as the explicit and implicit integrations; the time-dependent variables are

discretized using a finite difference technique via a time increment to estimate the continuous field variables in the next time step. By choosing different finite difference techniques, such as the forward or backward finite difference estimates, an explicit or implicit integration scheme can be obtained. We used the implicit method (backward finite difference) to take advantage of unconditional stability of the method. Although implicit integration is supposed to be unconditionally stable for any arbitrarily chosen time step, there are limitations due to considerations of numerical convergence and computational accuracy. This means that the time step must meet the Courant-Friedrichs-Lewy (CFL) condition for numerical stability. CFL condition represents Courant number $C = (|v|\Delta t/\Delta l) < 1$ in which, $|v|$ is the magnitude of the velocity vector (herein velocity of laser passing, which is equal to adding of the mass fraction to equations), Δt is time increment and Δl is a characteristic element length in the direction of flow. Due to the limitation that heat cannot be convected across more than one element length, Δl , within a single time increment, the transient temperature behavior is affected. Figure 39 (a, b) provides illustrations of the transient temperature at a specific point for two different times, while maintaining the same spatial discretization. In Figure 39 (a), the mesh size is set to 0.2 mm with a time step of 0.02 s. Conversely, Figure 39 (b) represents the same mesh size but with a smaller time step of 0.001 s. These figures aim to highlight the importance of the Courant-Friedrichs-Lewy (CFL) number, which is highly recommended. By selecting a CFL number less than 1, it becomes possible to predict the temperature variation over time without spurious oscillations. Even when using automatic time incrementation in the solver to ensure convergence, it is crucial to fulfill additional considerations to avoid such oscillations. The presence of these oscillations emphasizes the significance of carefully managing the time step and mesh size in order to accurately capture the transient temperature behavior during the simulation. The Peclet number is another dimensionless parameter that indicates the degree of convection dominance over mass adding to the computation domain and needs to be considered in AM process modeling, especially at the level of high-fidelity models. Figure 39 (a, b) also show the number of iterations required to achieve convergence in each increment, superimposed on the temperature versus time response.

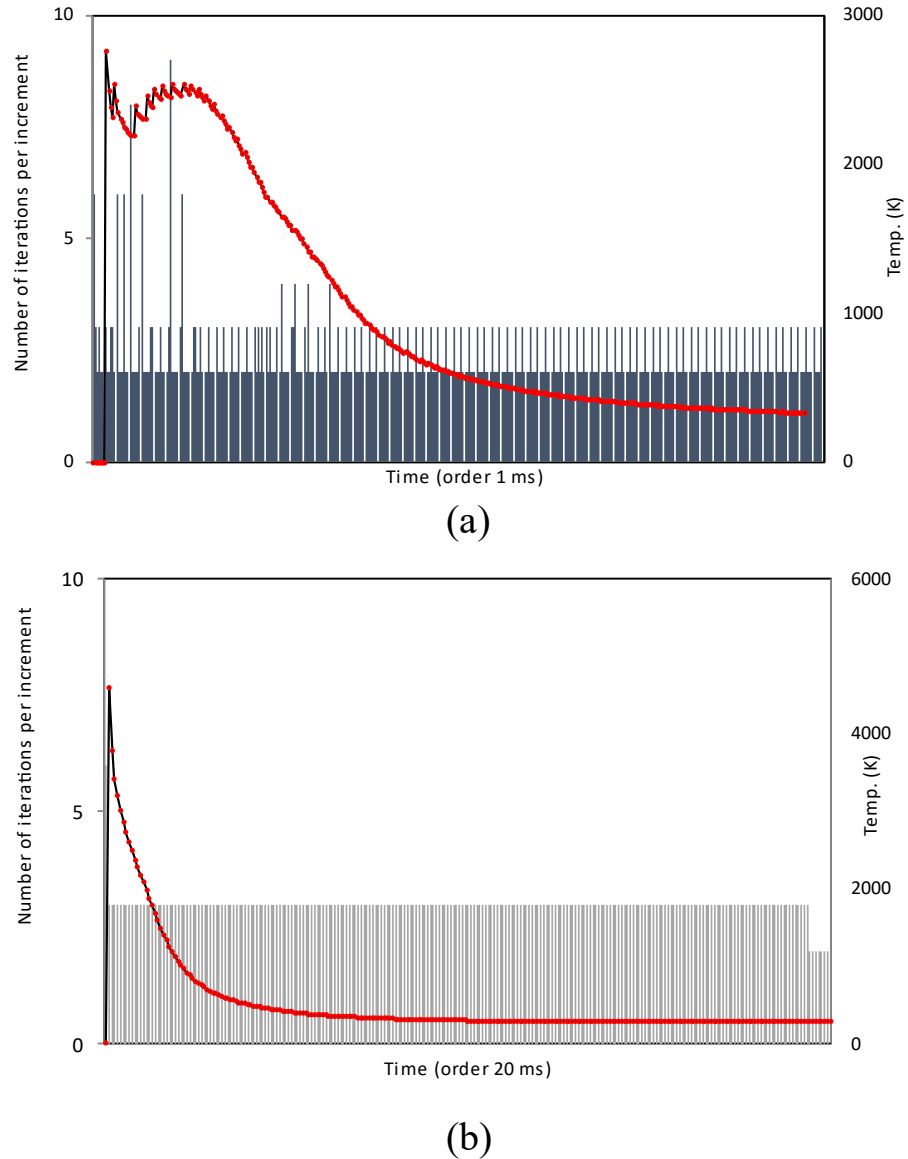


Figure 39 Transient solution of temperature for single line, number of iterations per increment, with the temperature versus time curve superimposed, (a): Mesh size 0.02 mm and time increment 0.001 s, (b): Mesh size 0.02 mm and time increment 0.02 s.

6.1.3.3.Characteristics of Melt Pool

The unique microstructures observed in additive manufacturing (AM) processes are primarily influenced by localized high thermal gradients and rapid cooling rates during solidification. In Figure 40 (a), temperature distribution profiles are depicted in relation to the distance from the head to the tail of the melt pool domain. The cooling rate is presented within the same time frame and calculation frame in the axisymmetric view. Within the molten isotherm domain at the center of the melt pool, the cooling rate approaches zero. In the head of the melt pool, near the region where new mass (powder particles) is added, a positive cooling rate is observed due to the mixture of powders and substrate (forming the mushy area with $0 < \psi < 1$). At the tail of the melt pool, a negative cooling rate indicates the initiation of solidification.

The Marangoni effect, arising from surface tension gradients, significantly impacts microstructure formation during additive manufacturing. While the computational model considers heat transfer through conduction, the temperature gradient perpendicular to the laser movement drives fluid motion within the melt pool. Depending on temperature variations, the melt pool exhibits upward or downward movement. These dynamics, attributed to thermal gradients and surface tension variations, play a crucial role in shaping the final product. In Figure 40 (b), localized laser heating creates a temperature gradient, affecting the melt pool's width and morphology.

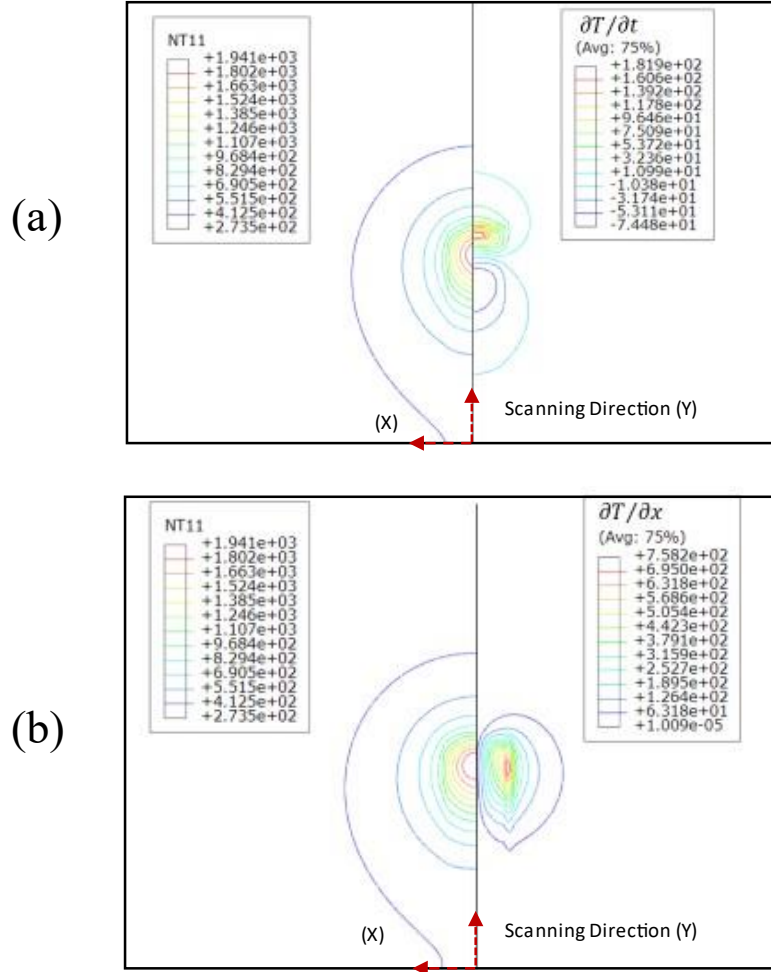
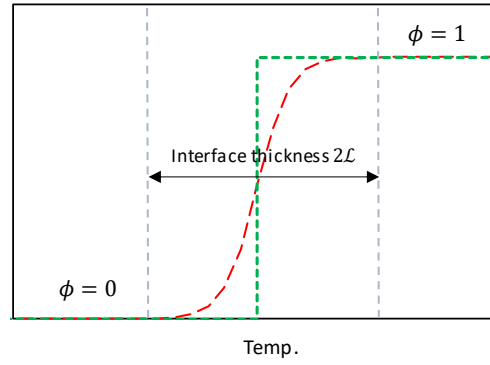
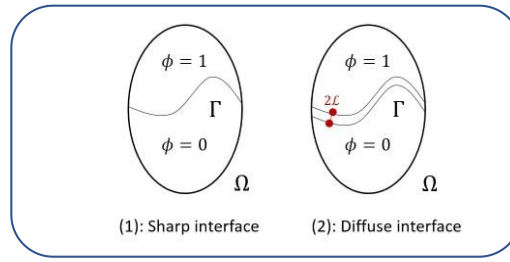


Figure 40 Top surface temperature sequence during AM process, (a): axisymmetric temperature view vs cooling rate taken at the same time frame, (b): axisymmetric temperature view vs temperature gradient taken at the same time frame.

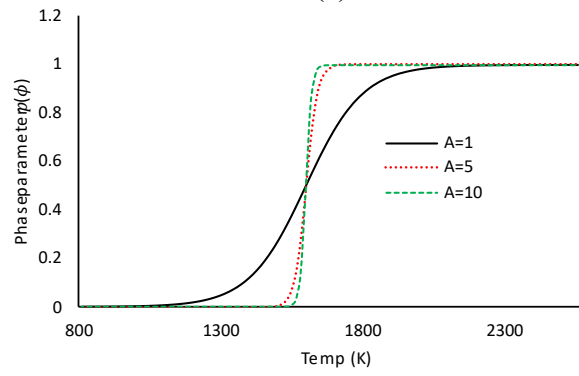
6.1.3.4. Effect of Phase Change on Enthalpy

Here, we focus on addressing the phase change problem, specifically the transition from powder to the molten phase and subsequently from the molten to solid phase during the deposition process in additive manufacturing (AM). We consider domains that encompass the phases existing between the powder and molten state, as well as the molten and solid state, with an interface separating them. Two primary models are utilized to describe the phase change process, namely

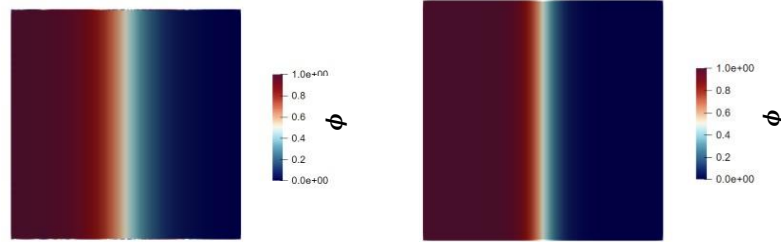
the sharp interface model and the diffusive interface model, as depicted in Figure 41 (a, b). In the sharp interface model, the initial assumption is that the solid and liquid phases are separated by an infinitesimally thin interface determined by temperature. However, accounting for this sharp interface properly in numerical processes using a Lagrangian description poses challenges. Nonetheless, in an Eulerian description, when combined with explicit interface tracking schemes such as level set functions [145], the sharp interface model can be applied. In our approach, we employ a model where the phase change occurs across an extended interface domain with a finite thickness, employing a latent heat model. The transition between phases is extensively explained in Chapter 4, and the impact of the steepness in the phase function parameter is illustrated in Figure 41 (b). To overcome the nonlinearity phenomena in the AM process, we generally utilize a larger transition region in our proposed model. Figure 41 (b) demonstrates that in a Lagrangian description, as A approaches infinity, a diffusive function can be employed to approximate a sharp transition condition based on Equation 4.42. The enthalpy function for a material point is extracted from the developed code in ABAQUS and depicted in Figure 42. The slope of the function represents the specific heat for the liquid and solid phases, while L_f denotes the latent heat of fusion. In the mushy region, average specific heat values are utilized. These values are based on the description provided in reference [146].



(a)



(b)



(c)

(d)

Figure 41 Phase transition, (a): two approaches of sharp interface and diffuse interface with the phase field function ϕ in domain of temperature, (b): Effect of sharpness of transition in phase function interpolation, effect of sharpness of transition in interface reaction, (c): $A = 5$, (d): $A = 10$.

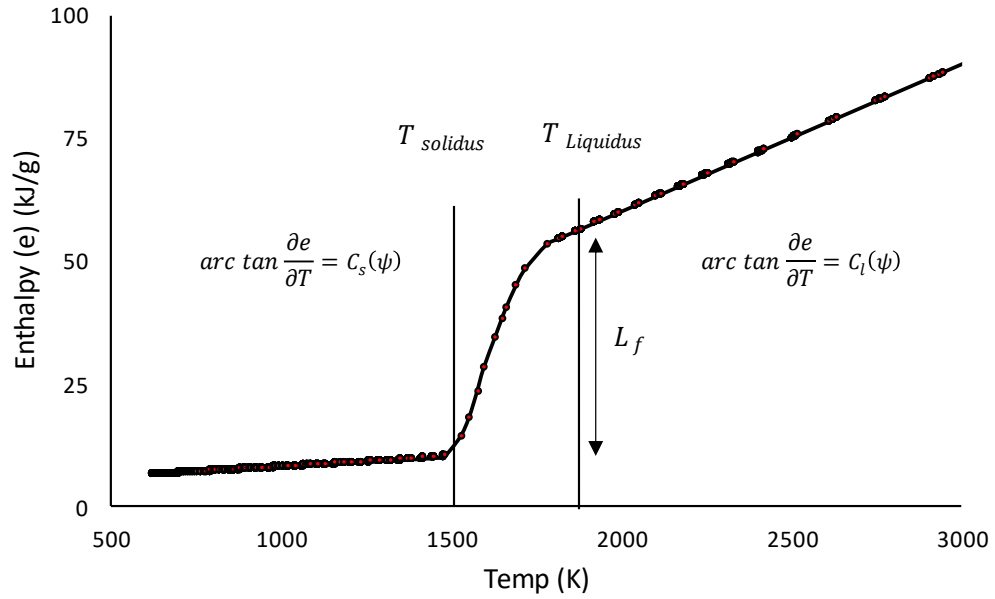
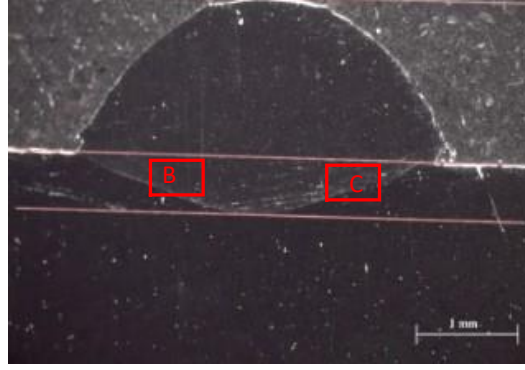


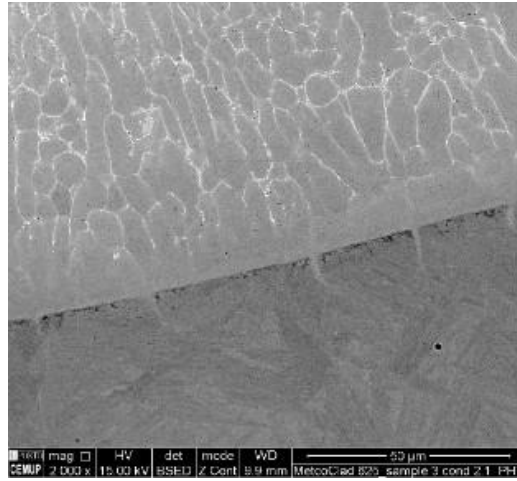
Figure 42 Temperature dependent specific enthalpy for material point in ABAQUS.

6.1.3.5. Local temperature gradient and solidification rate

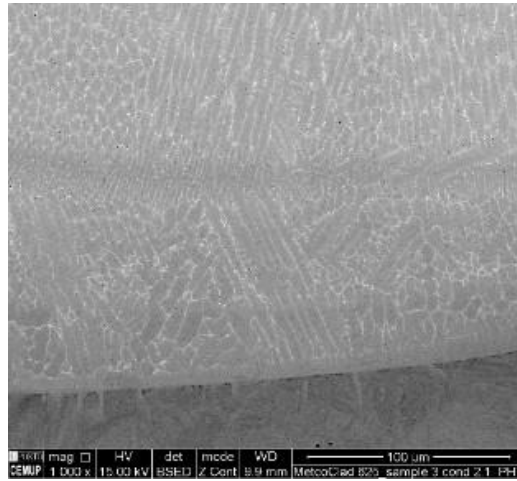
The temperature gradient G and solidification growth R are the most significant parameters in determining the solidification microstructure (e.g., planar, cellular, columnar dendritic, and equiaxed dendritic grain structure). A solidification micro graphical map for Inconel 625 on 42CrMo4 demonstrating the variation in the morphology and size is presented in Figure 43 (a-c). As can be seen, the dendrite morphology, orientations, and micro segregation are different at different locations within the melt pool. This is primarily due to different positions and orientations of the initial nuclei combined with different thermal gradients and solidification velocities along the melt pool boundary.



(a)



(b)



(c)

Figure 43 (a) Optical micrograph demonstrating transverse cross-sections of melt pool obtained under $P = 2 \text{ kW}$, $SS = 10 \text{ mm/s}$, $FR = 15 \text{ gr/min}$, (b) ,(c) enlarged views.

In the presented model, $\mathbf{G}$ represents the gradient vector of temperature with respect to each Cartesian coordinate. The norm of the gradient vector, denoted as $\|\mathbf{G}\|$, can be calculated using Equation 6.6:

$$\|\mathbf{G}\| = \sqrt{G_x^2 + G_y^2 + G_z^2} \equiv \sqrt{\partial T_x^2 + \partial T_y^2 + \partial T_z^2} \quad (6.6)$$

On the other hand, the growth rate, denoted as R , is derived geometrically by projecting the laser velocity vector, denoted as $\mathbf{v}$, onto the normal vector of the solidification front. This projection is determined by the angle θ , which represents the local angle between the surface normal to the liquidus isotherm boundary and the welding direction. Equation 6.7 and Figure 44 illustrate the calculation of the growth rate as:

$$R = \|\mathbf{v}\| \cos(\theta) \quad (6.7)$$

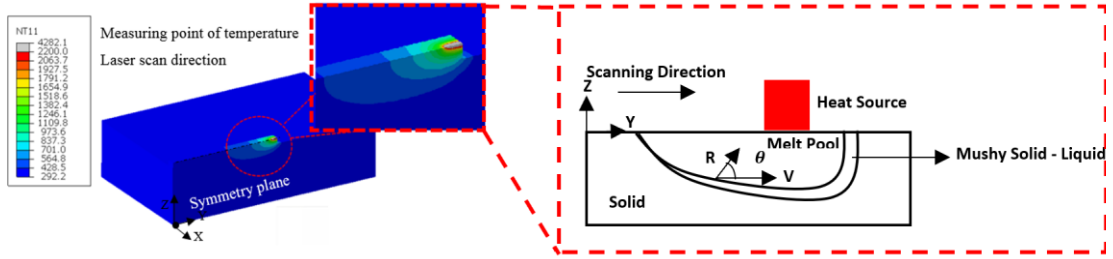


Figure 44 Schematic of solidification growth rate R in the melt pool with laser scanning V .

The values of $\mathbf{G}$ (gradient vector) and R (growth rate) were obtained from macro-scale simulations. Points of interest were selected along the trailing half of the melt pool, which represents the region undergoing solidification. Figure 45 (a, b) illustrates the variation of $\|\mathbf{G}\|$ and R along the centerline of the melt pool boundary as the depth increases. The results indicate an inverse relationship between R and $\|\mathbf{G}\|$. The maximum value of R is observed near the top of the melt pool, where the solidification front depth is low. Conversely, the minimum R is found near the bottom of the melt pool, where the solidification front depth is high. In contrast, the maximum $\|\mathbf{G}\|$, is calculated at the bottom of the melt pool, while the minimum $\|\mathbf{G}\|$, is observed at the top. The bottom region, characterized by high $\|\mathbf{G}\|$, and low R , corresponds to planar grains as depicted in Figure 43 (b), which is supported by SEM microstructure evidence. On the other hand, the top regions exhibit relatively lower $\|\mathbf{G}\|$, and higher R , resulting in a dendritic structure as shown in Figure 43 (c).

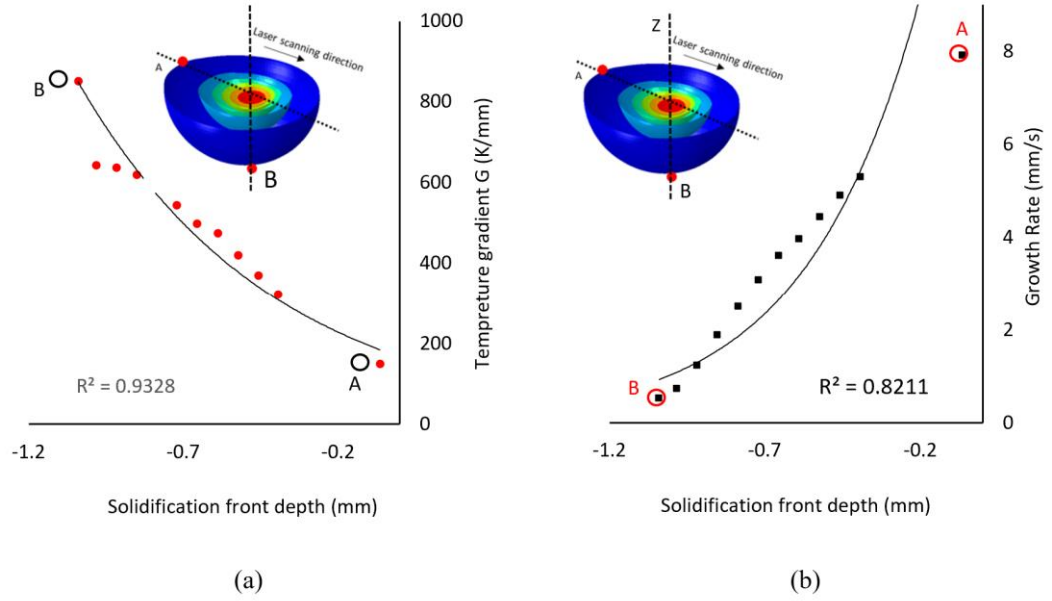


Figure 45 The calculated (a): $\|G\|$, and (b): R , along the centerline of the melt pool surface; Variation in relation with the solidification front depth for one set of parameters $P = 2 \text{ kW}$, $SS = 10 \text{ mm/s}$, $FR = 15 \text{ gr/min}$.

Figure 46 (a,b) illustrates the cooling rate for two set of parameters including (a): $P = 2 \text{ kW}$, $SS = 10 \text{ mm/s}$, $FR = 15 \text{ gr/min}$ and (b): $P = 1.5 \text{ kW}$, $v = 10 \text{ mm/s}$, $F = 15 \text{ gr/min}$. It can be observed how the cooling rate, $\dot{T}$, varies as a function of the melt pool depth for both cases. The dotted rectangular views emphasize the highest and lowest cooling rates, along with the location of the melt pool boundary. Simulation results show that the cooling rate increases from bottom to top along the melt pool boundary. Additionally, the predicted cooling rate varies with changes in the laser power. Specifically, the cooling rate increases with decreasing laser power [147][148], leading to a variety of solidified microstructures

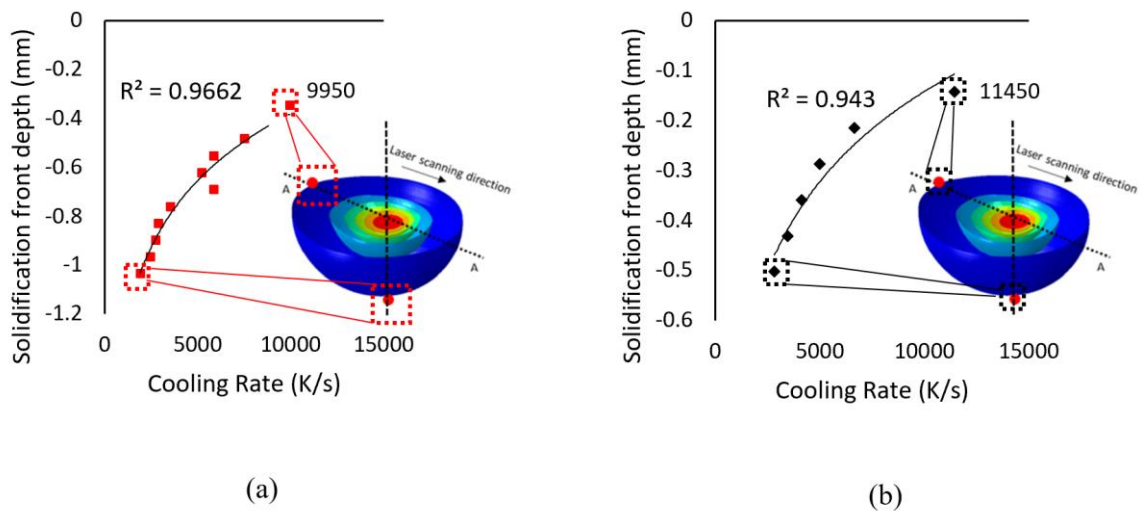


Figure 46 The predicted cooling rates at varying solidification front depths for two sets of process parameters; (a) $P = 2 \text{ kW}$, $v = 10 \text{ mm/s}$, $F = 15 \text{ gr/min}$, (b) $P = 1.5 \text{ kW}$, $v = 10 \text{ mm/s}$, $F = 15 \text{ gr/min}$.

6.1.3.6. Residual Stress and Strain of single track

The thermal history obtained from the heat transfer analysis is applied to the mechanical analysis to evaluate residual stress and strain distribution as function of time. The temperature-dependent material properties for Inconel 625 solid are given in Figure 29 (a-g). For powder and liquid states, the material's stiffness is negligible compared to the stiffness of the dense solid state. Thus, a small value (0.1 GPa) compared to the value of the dense solid-state under room temperature (213 GPa) is used for the powder stiffness to make it virtually zero (deactivated) but not exactly zero to guarantee a positive definite stiffness matrix in the solution. The negligible yield stress at the melting temperature is set to be 0.1 MPa assuming perfect plasticity to consider the annealing effect (equivalent plastic strain is reset to zero to remove the hardening memory) [149] at the liquidus temperature. The controlling of the time increment for the thermal analysis is described in section 6.1.3.2. For the mechanical analysis the same time increment can be used but is not ideal when the problems are highly nonlinear. In this approach, a mechanical time increment that is five times larger than the thermal time increment is allocated to the mechanical analysis. This allocation is done in order to optimize computational resources. The rapid temperature decrease following solidification has minimal impact on stress evolution due to the low elastic modulus values at high temperatures. Figure 47 presents the evolution of transverse stress and longitudinal stress at the midpoint P of the cladding as a function of temperature for the specified point. At the initial stage of laser cladding, the coating formed is heated to expand and extrude the unreformed part, which makes the longitudinal stress develop into compressive stress at first, and at the same time, the coating center is heated to expand freely in the transverse direction to form tensile stress. Throughout the melting of cladding, both transverse and longitudinal stresses are close to the unstressed state while decreasing temperature leads to solidification and stress evolution starts to develop compressive stress in 0.45 s . After the coating is completely cooled down to ambient temperature, the longitudinal and transverse stress stabilize at about 665.63 MPa and 166.8 MPa respectively. Figure 48 (a-c) shows the transverse, longitudinal and von Mises residual stresses for single track computational domain. In triple cases the maximum tensile stress are around $800\sim 900 \text{ MPa}$ and compression range of -700 MPa . The transverse compressive stress in the middle of the substrate was caused by the shrinkage of the substrate pulled by the shrinkage of the cladding solidification (Figure 48 (a)). It is well documented by [150,151] that high tensile stress at the junctions of cladding and substrate is one of the main reasons for induced cracking. In Figure 49, all components of stresses for a cross-sectional path show that the stress trend changes from the top of the coating to the top surface of the substrate, changing from tension to compression. Overall, the surface of the substrate is in a low transverse stress state and gradually transits to tensile stress toward the coating. The tensile stress can be seen reaching its maximum at the junction of substrate and cladding.

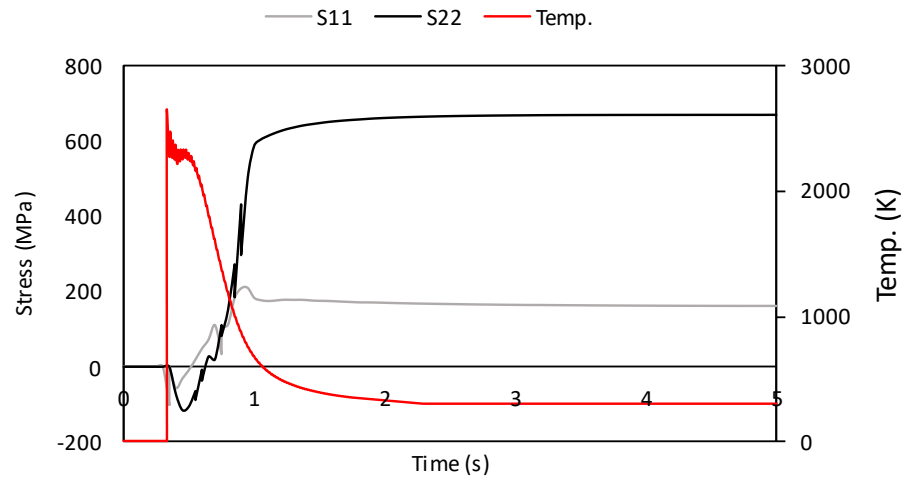
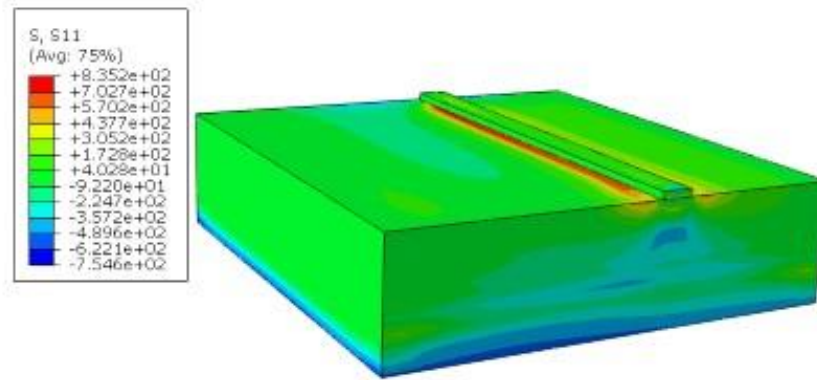
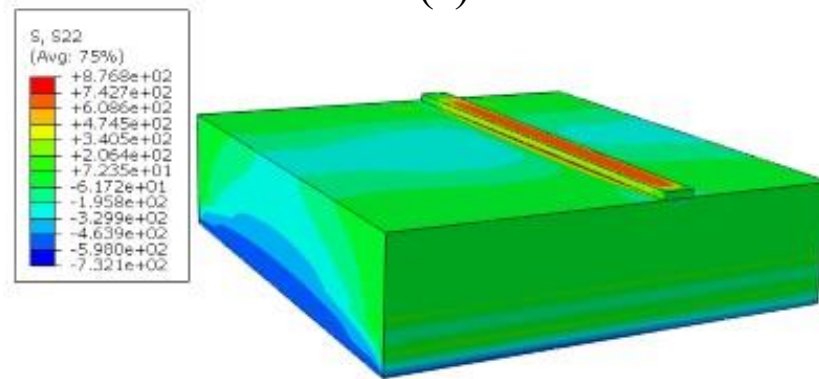


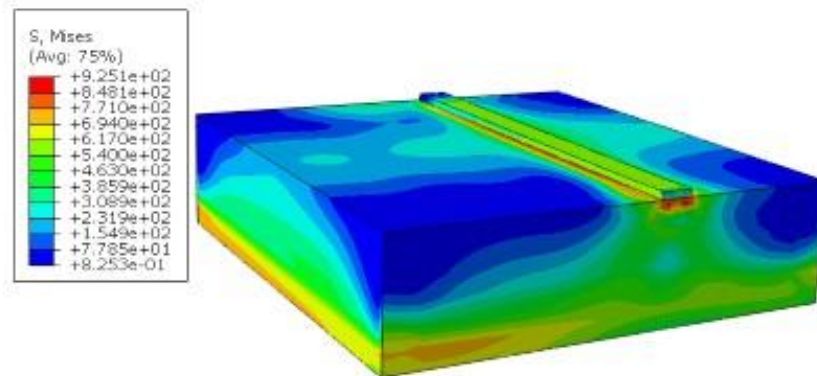
Figure 47 Stress evolution at midpoint P ; transverse stress (S11) and longitudinal stress (S22) against time accompany of temperature distribution



(a)



(b)



(c)

Figure 48 Residual stress evolution (a): transverse stress (S11) and (b): longitudinal stress (S22), (c): equivalent Mises stress.

Stresses are all in MPa.

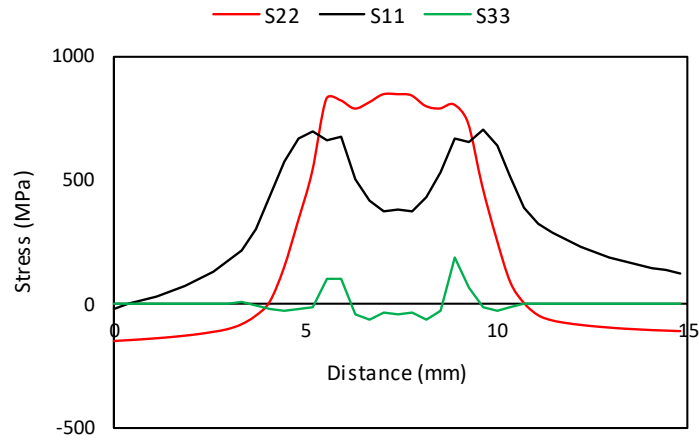


Figure 49 Longitudinal and transverse and radial stresses distribution along cross-sectional view

6.1.4. Multi-Layer Scale

In this section, a direct energy deposition (DED) system equipped with a robot (Kuka, Augsburg, Germany) was utilized to fabricate a thin-walled multi-layer tracks structure, as depicted in Figure 50 (a). Table 6 show the process deposition parameters to be used for the simulation stage. Numerous continuous layers of Inconel 625 powder were deposited with an inter-pass time of 0 (s). In order to build the structure layer by layer, the metal fabrication procedure follows the pattern that is depicted in Figure 50 (b).

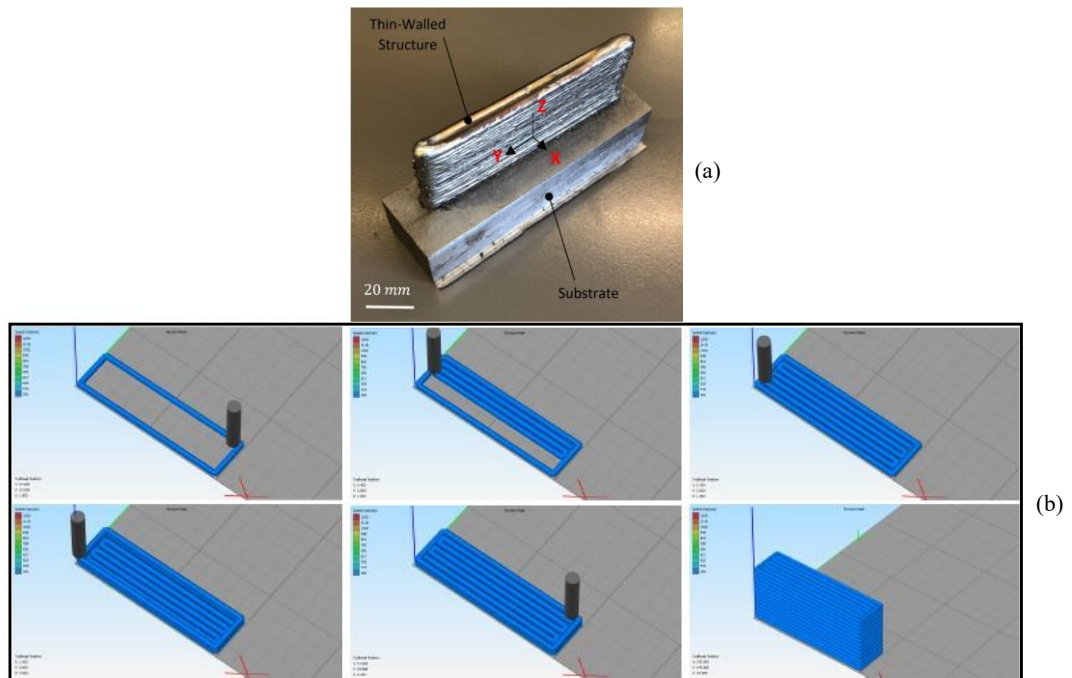


Figure 50 Manufactured thin-walled structure by DED process, (b): schematic of the filling-contour pattern during fabrication in DED (Not-True-Scale).

Table 6 DED manufacturing process parameters

Hatch Spacing (mm)	Layer thickness (mm)	Laser spot size (mm)	Laser Power (kW)	Feed rate (g/min)
1.8	1.7	2.5	1.8	12
Scanning Speed (mm/s)	Shield Gas Rate (L/min)	Carrier Gas Flow Rate (L/min)	Shield gas	Carrier gas
6	26	2.5	Argon	Argon

6.1.4.1. Thermal Prediction at the Multi-Layer Scale

In this section, a thermal simulation of a multi-layer structure to fabricate the thin-walled structure is conducted to obtain the map of temperature, cooling rate, and phase-field parameters on the FE nodes. The main idea is to expand the considerations of single-layer scale modeling to the multi-layer case to cover the effect of re-solidification for further studies like residual stresses. Upon the laser source movement, the surrounding nozzles simultaneously inject metallic powders into the laser beam and deposit them onto the substrate. The local heated point reaches rapidly the maximum temperature value. The material is added layer-by-layer and solidifies from the melt pool to create new features. The evolution of phase definitions based on local temperature in the DED process is illustrated in Figure 51 (a-c). The material state can be tracked using the adopted state variables in the developed code, namely ϕ and ψ . When both ϕ and ψ are equal to 0, the material is in a powdered state without being melted. As the powder absorbs sufficient energy, the material state transitions to a consolidated state with $\psi = 1$, as shown in Figure 51 (a). It is worth noting that between the powder and liquid states, there exists an intermediate condition known as the mushy powder-liquid state, where $0 < \psi < 1$. As the heat source moves, the material first melts with $\phi = 1$, and then solidifies after cooling with $\phi = 0$. The liquid state and bulk solid state are both considered as a dense state with $\psi = 1$. As the temperature changes, the porosity transitions to a solid state. Figure 51 (c) illustrates the variation in porosity within the melt pool and after solidification. It is expected that when powder particles are molten, no porosity remains between the particles, and the macroscopic porosity value ε is given by $\varepsilon = \varepsilon_0(1 - \psi)$, which varies with temperature. It is worth noting that the multi-layer model utilizes lumped resolution to save computational costs. The inclusion of phase change and material status highlights the model's capability in detecting material phases and assigning phase-dependent material properties during the process simulation. This enables a more accurate representation of the material behavior during the modeling process.

As shown in Figure 52 (a-c), two nodes, labeled A and B, are selected as points of interest to study temperature and phase evolutions in the fabricated thin-walled structure. The temperature profiles exhibit sharp peaks, indicating rapid heating and cooling cycles as the laser scans over the nodes within a short time frame. Point A experiences a lower peak temperature compared to point B, which can be attributed to heat accumulation during the deposition of middle layers.

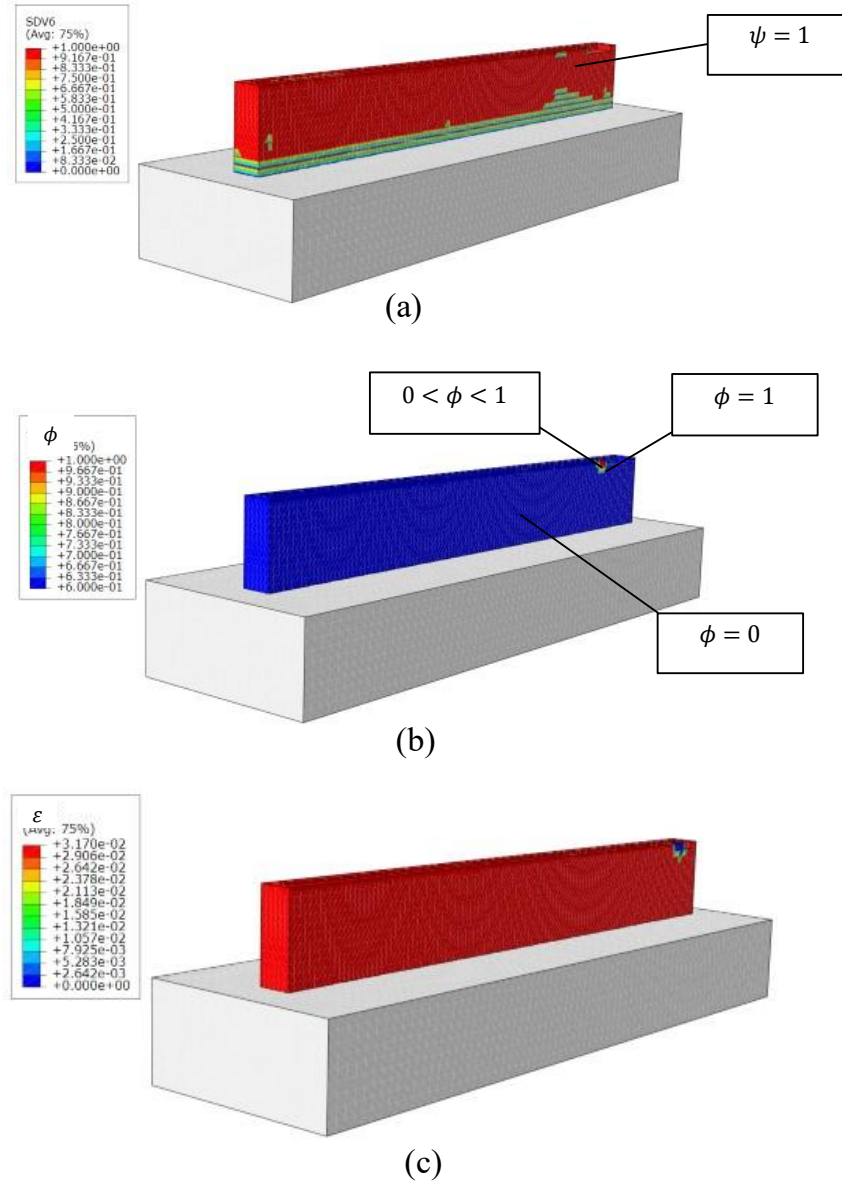
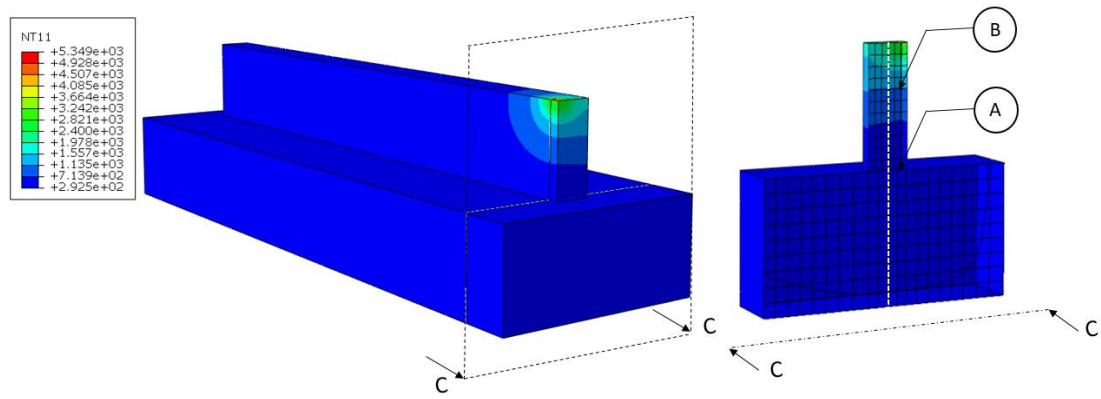
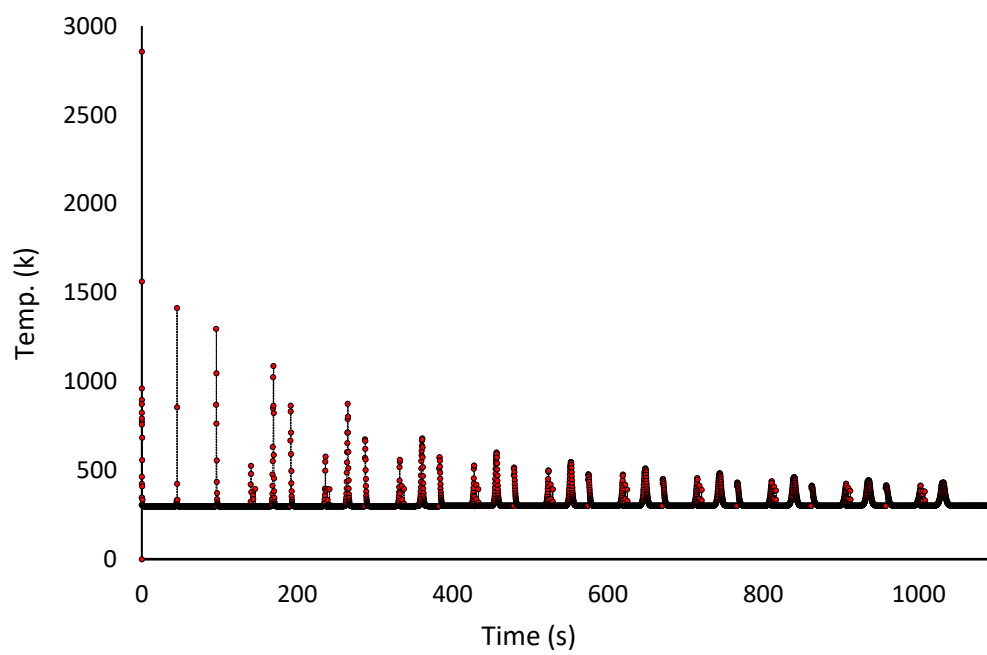


Figure 51 Prediction of phase domain in-situ printing of the thin-walled structure; (a): consolidation control to record history the melted FE nodes, (b): liquid-fully solid phases for FE nodes, (c): porosity evolution.



(a)



(b)

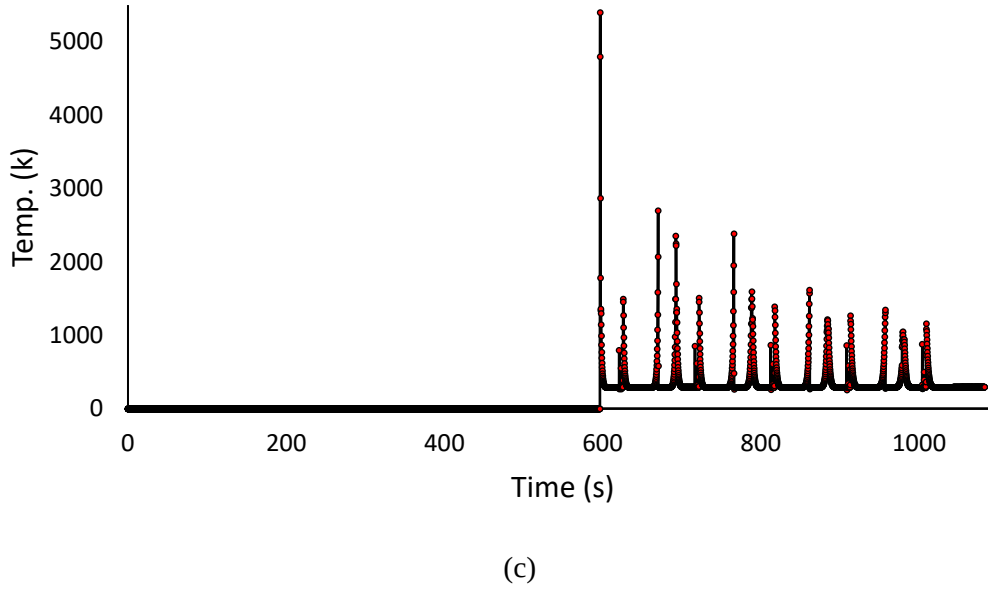


Figure 52 Transient temperature field and state variables for a point of interest A; (a): Temperature contour in the thin-walled and sectional view of the area contains A Point, (b): Temperature vs time for point A, (c): Temperature vs time for point B.

6.1.4.2. Residual Stresses Prediction in the Multi-Layer Scale

In this section, the single-layer residual stress considerations are adopted for the prediction of residual stress and distortions in the multi-layer case study. As explained in Chapter 4, an uncoupled mechanical simulation is loaded, taking advantage of the thermal responses. In this simulation, opposite to the utilized approach in the simulation of the single layer with various elements in the coating height domain, just one element is dedicated for an entire layer thickness, according to the research results in [26,152,153]. Those results showed that by increasing the number of elements in height, a sensitivity analysis revealed slight improvement while increasing computational cost significantly. The investigation of the temperature history reveals that the highest thermal gradient is around the vicinity of the heat source and that a non-symmetrical thermal profile in the structure leads to a very high cooling rate in the solidification process. The residual stresses are originated from thermal expansions between irradiated and surrounding material during phase change. Figure 53 (a-h) shows the three-dimensional stress components, including σ_{11} , σ_{22} in different stages of the deposition process after the first layer deposition, in the 50 percent of building direction, then 75 percent of deposition and finally covering the whole height of the thin-walled structure. When the material has a powder and liquid state, corresponding to a small modulus of elasticity, stresses are notably lower when compared to those within the solid-state region. In almost all stages of the process, the top surfaces are mostly dominated by minor tension stress and in the clamped surface at the bottom of the substrate, the highest value of compression stress can be seen. Therefore, a thinner substrate may lead to the

higher residual stress due to the greater constraints from the bottom surface. Against the tensile behavior of the topmost layers in all stages, there is a compression trend in the lower layers to satisfy the force and momentum equilibrium. The stress evolution in the transverse direction in the first layer illustrates that the strongest gradient belongs to the interface between the part and substrate and then shifts to the middle of the structure. The maximum longitudinal stress is on the exterior surface of thin-walled structure and, by the evolvement of the fabrication, remains in the half middle near the bottom.

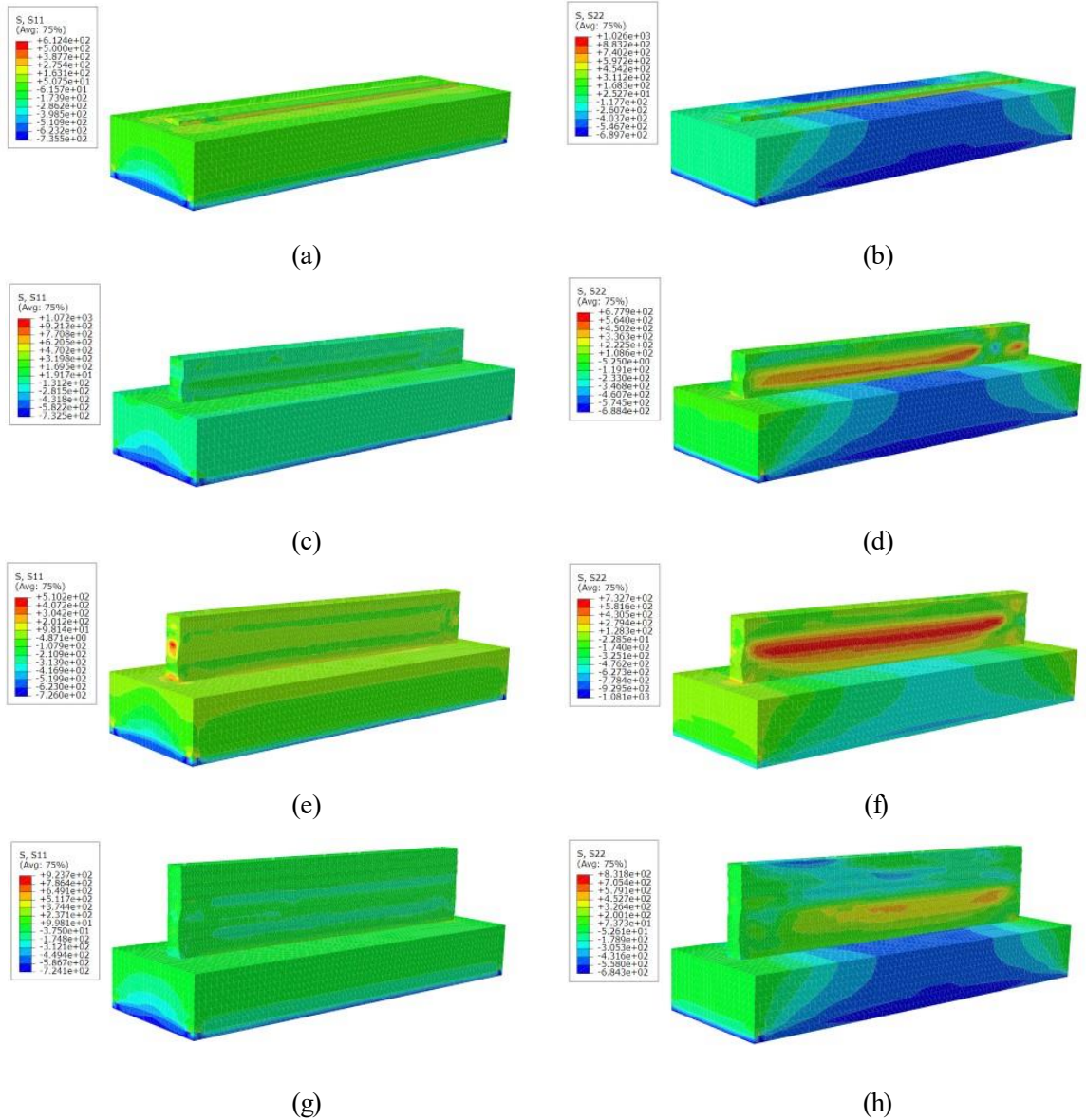


Figure 53 Stress distribution throughout the fabrication of thin-walled layer, (a): transverse stress in the first layer, (b): longitudinal stress in the first layer, (c): transverse stress in 50% of the height, (d): longitudinal stress in 50% of the height, (e): transverse stress in 75% of the height, (f): longitudinal stress in 75% of the height, (g): transverse stress in full height, (h): longitudinal stress in full height.

The subplots in Figure 54 (a-d) display the Von-Mises stress evolution throughout the deposition process. The pick stress progression is located at the bottom of the substrate and can be seen after accomplishing the process. The maximum value locates on the lateral surface.

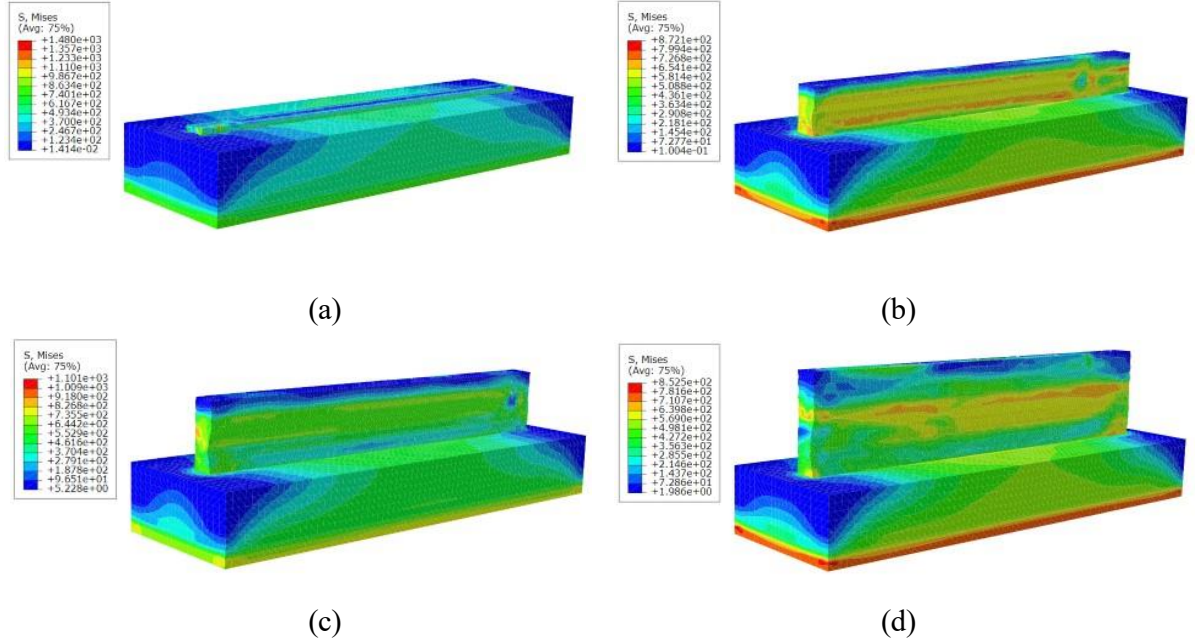


Figure 54 Simulated Von Mises stress distribution throughout the fabrication of thin-walled layer, (a): the first layer, (b): in 50% of the height, (c): in 75% of the height, (d): in full height.

The graph in Figure 55 illustrates the predicted internal residual stress evolution at the height of the fabricated thin-walled structure, from the bottom in interaction with the substrate to the top point of the last layer after cooling down. The detailed view of the selected cross-section in the middle of the structure was shown inside the graph. The stress evolution shows that longitudinal stress steers the deformations more than the other two components, and it can be concluded that deformation reduction can be obtained by reducing the longitudinal stress effect.

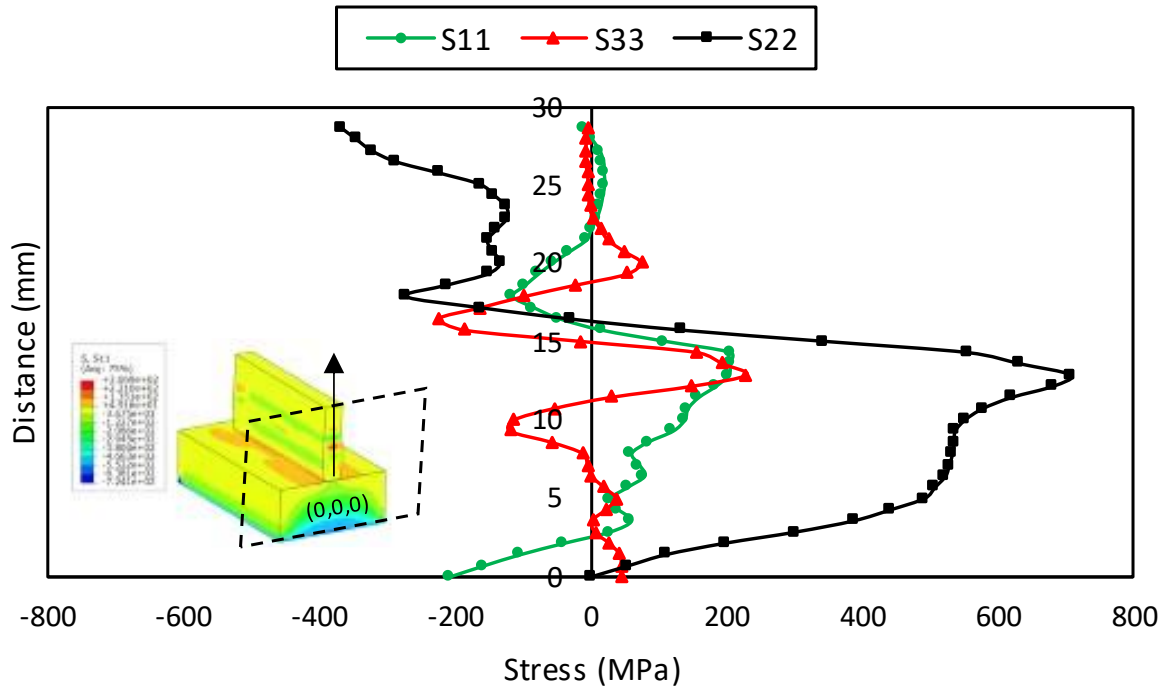


Figure 55 Predicted components of the residual stress in the center line of the middle cross-section plane in the thin-walled structure.

The comparison of the temperature history field for both points in Figure 52 (a-c), in the first layer near the external surface and in the middle of the structure show that heat accumulation leads to the increase of the peak temperature in the middle of the structure. Furthermore, the heat accumulation governs the pool volume increase slightly while the stiffness drops for these layers because of the higher temperatures. Therefore, the displacement value increases continuously from the bottom to the middle and then slightly changes when reaches the topmost layers. In Figure 56 (a-d) the progressive process shows that the maximum displacement is in the middle of the wall near the substrate because the middle layers are under repetitive melting and re-solidification cycles. Evidence illustrates that by reaching the top, the displacements are getting a more stable trend due to losing temperature by convection and radiation. The peak displacement in the middle of the wall originates from a repetitive laser trajectory with identical start and end points for all layers. This leads to an evident twisting effect in the middle part, as shown in Figure 57 (b). This finding highlights the crucial significance of carefully designing the trajectory, both in the filling and contouring processes. In another attempt in catching the border of ideal and deformed shapes in Figure 57 (a), explicitly it can be concluded, as expected, that thin-walled taller structures are more susceptible to deformation than the shorter ones. Herein, it can be emphasized that there is a critical need to have robust procedures in designing the thickness and height of thin-walled structures, in correlation with the scan trajectory and even dwell time.

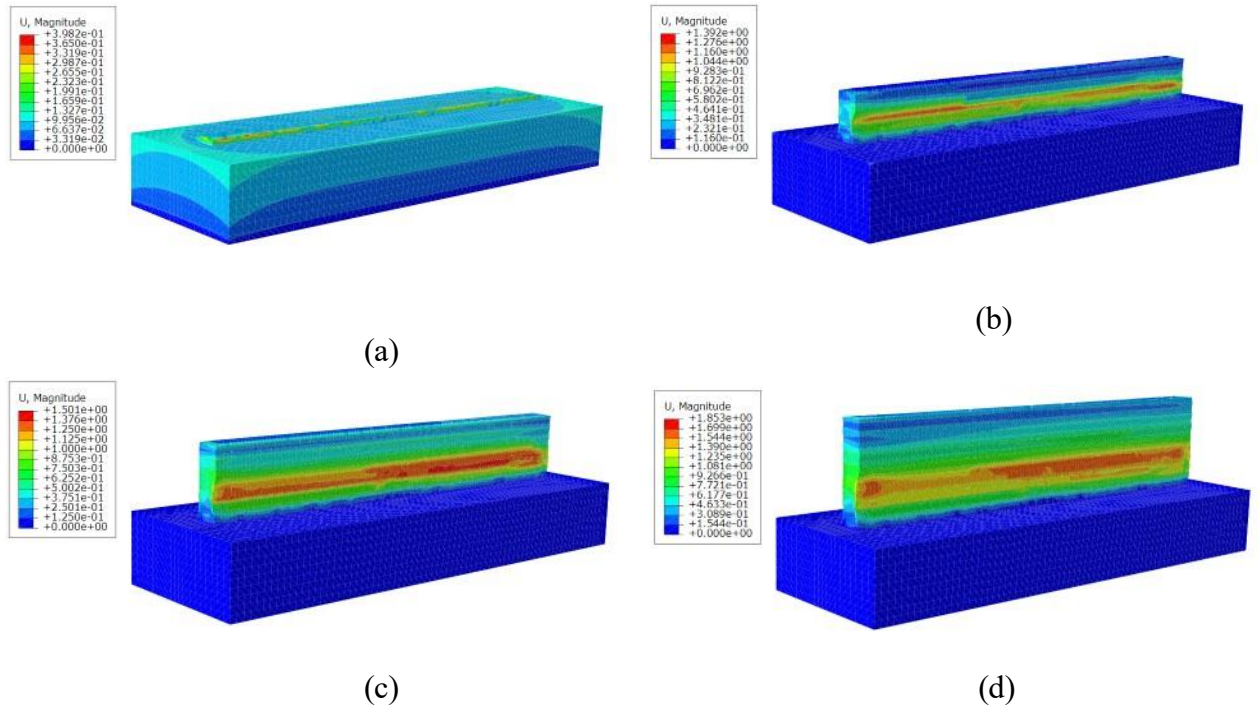


Figure 56 Total displacement throughout the fabrication of thin-walled layer, (a): the first layer, (b): in 50% of the height, (c): in 75% of the height, (d): in full height.

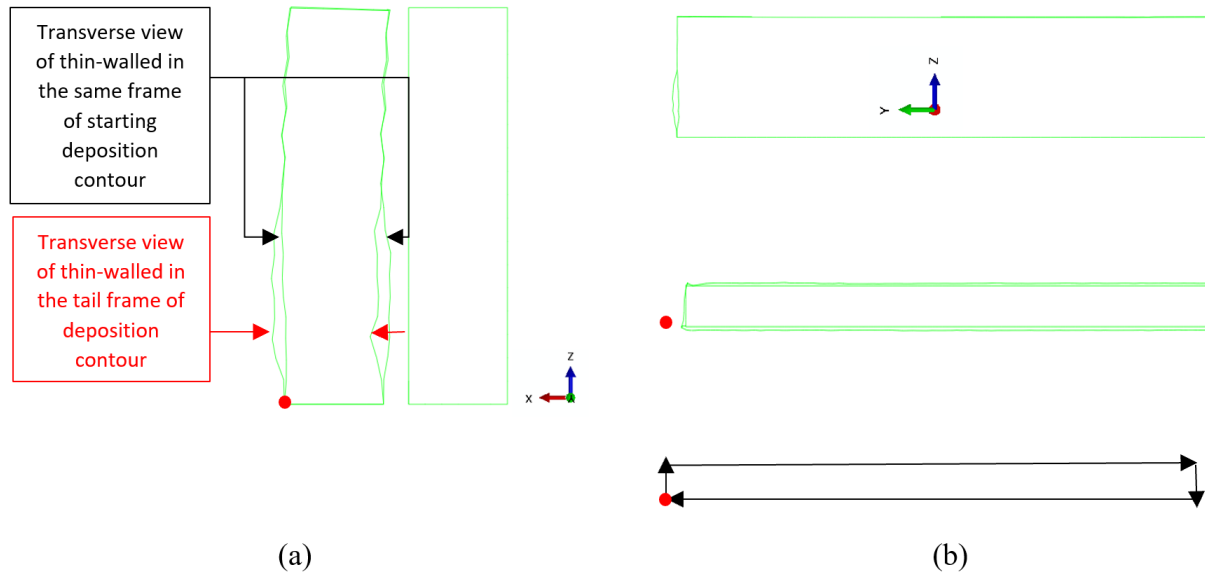


Figure 57 Comparison of the deformed and unreformed edge of thin-walled structure induced by thermal and mechanical loads, (a): in transverse sectional view, (b): in longitudinal and top sectional views.

6.1.4.3. Effect of the melt pool size on the solidification and microstructure

The cooling rate is the product of the temperature gradient (G) and solidification growth rate (R): $\dot{T} = G * R$. Figure 58 illustrates the reference solidification map. The ratio of these parameters, G/R , determines the morphology of the solidification microstructure (e.g., planar, cellular, columnar dendritic, and equiaxed dendritic). A consequence of the cooling rate is the size of the microstructure, meaning that the higher the cooling rate, the finer the microstructure [24].

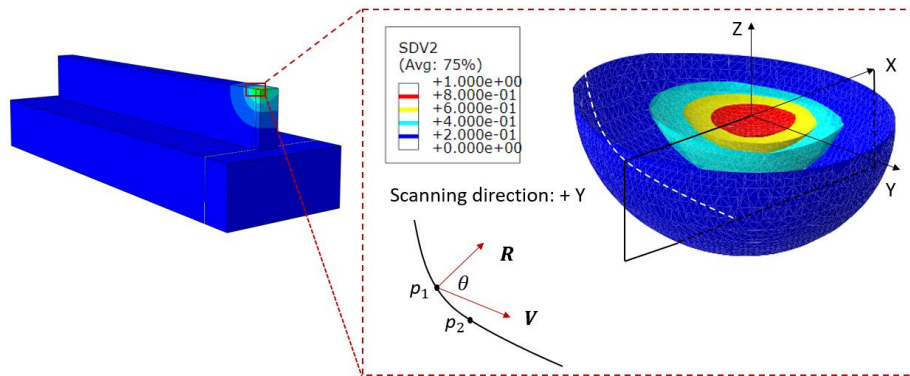


Figure 58 Schematic diagram of melt pool and associated variables and axes used in the analysis in a Cartesian system.

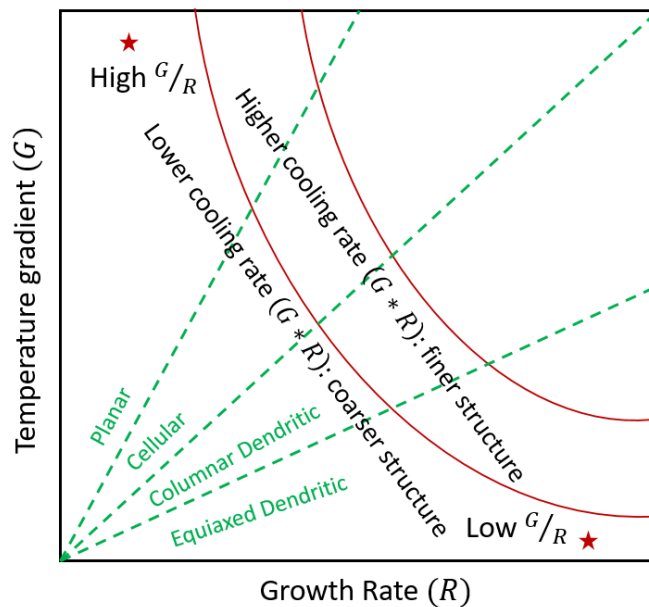


Figure 59 Temperature Gradient G and Liquid-solid interface velocity R in a plot as a reference solidification map.

In Figure 60 a comparison on the melt pool size in layers *C* and *D* reveals that the melt pool dimension increases steadily until it levels up due to accumulating the temperature in the printed wall, with a weaker heat dissipation. Moreover, as revealed in Figure 60, the peak temperature in the topmost melt pool increased considerably while the solidification rate noticeably decreased in comparison with the bottom region. That means the solidification at the topmost region (*C*) takes longer than that of the bottom region (*D*). This temperature difference between *C* and *D* influenced the grain size formation.

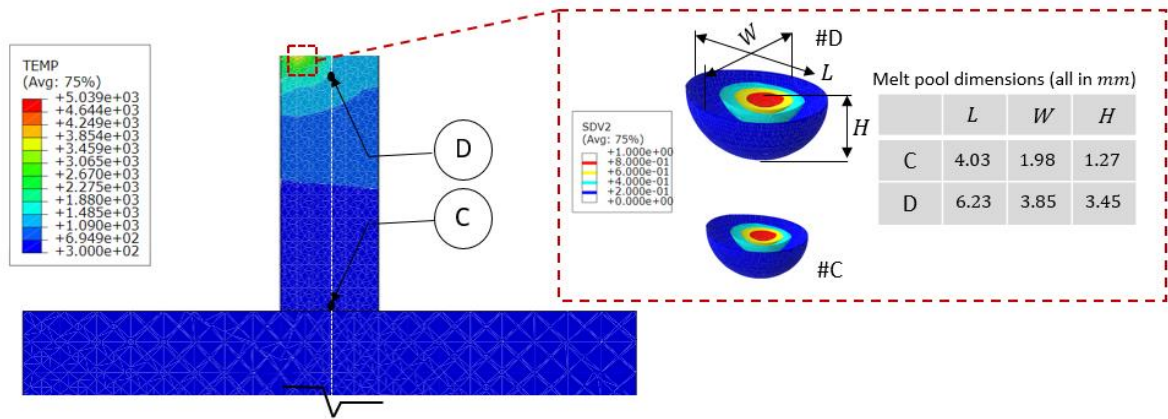


Figure 60 Melt pool variations throughout process for two points *C* and *D*.

A transversal cross section specimen was prepared from the printed wall seen in Figure 50 (a), applying conventional metallographic techniques. The zones of interest for microstructural observations represent the wall's centre line near the substrate and close to the top of the printed material, respectively indicated as *C* and *D* in Figure 60. The microstructural observations (Figure 61 (a-d)) were performed using an optical microscope Leica DVM6 A, using LAS X version 3.014 software, and a scanning electron microscope (SEM), an FEI Quanta 400 FEG (ESEM, Hillsboro, OR, USA) equipment. Microstructural assessments involved local chemical analysis and crystallographic evaluations respectively conducted by energy-dispersive X-ray spectroscopy (EDS), EDAX Genesis X4M Oxford Instrument, and electron backscatter diffraction (EBSD), EDAX-TSL OIM detector and TSL OIM Analysis 5.2 software. Moreover, the microhardness measurements were performed on similar zones by a ZwickRoell & Emco-Test DuraScan 10/20 G5 applying 300 gf indentation (H V0.3). As seen in Figure 61, the grains are much smaller at the bottom of the fabricated wall than at the topmost region.

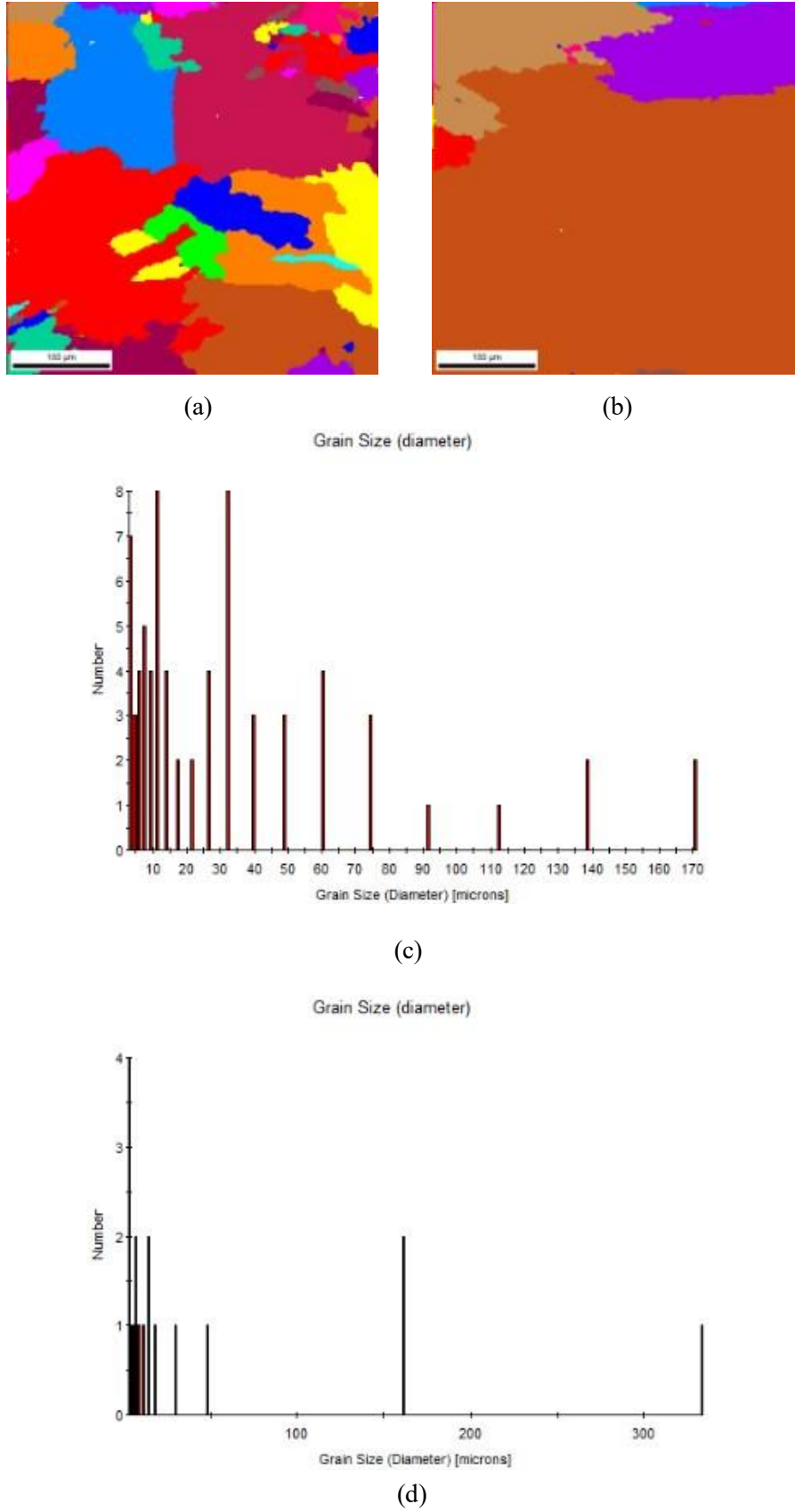
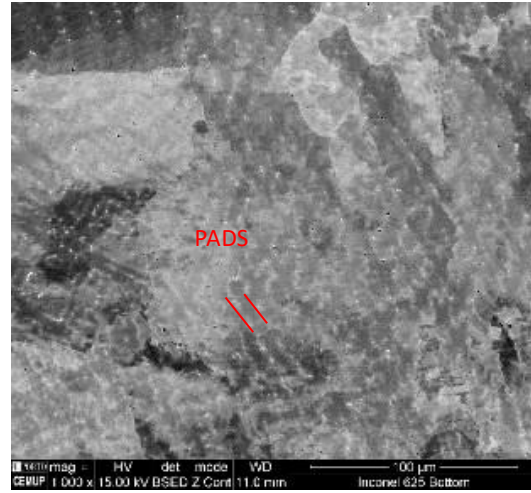
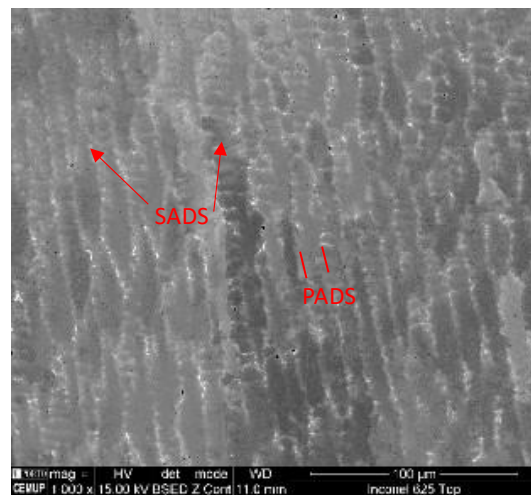


Figure 61 The grain size evolution in the deposited 625 alloy by DED in the XZ cross section studies by EBSD analysis: (a), (b): grain maps of the point C, D respectively, and (c), (d): grain size distribution in the similar zones.

The dendritic growth theory indicates that the average primary dendrite arm spacing, (PDAS), ($\bar{\lambda}$) has an approximate relationship with the growth rate (R) and thermal gradient (G), which means that $\bar{\lambda} \propto R^a * G^b$, a and b are constants associated with alloy [154]. It can be seen in Figure 62 (a, b) that the average PDAS increased from the bottom zone to the top zone in the deposited wall, or, in the other words, by increasing the cooling rate ($\bar{\lambda}$) decreases. The temperature gradient in D is greater value than in C, whereas the maximum solidification rate has a reverse trend in those two points. As seen in Figure 62 (a, b), the microstructure in the bottom region, point C, is constituted by dendrites with a smaller PDAS than that of the top region as in point D. As it is seen in Figure 62 (a, b), by increasing the deposition height, secondary dendrite arm spacing (SDAS) gradually appears, due to being exposed to subsequent thermal cycling and heat accumulation, which is proved in section 6.1.4.1.



(a)



(b)

Figure 62 Microstructure in different zones of deposited Inconel 625, (a): C point, (b): D point.

6.1.4.4. Phase fraction predictions for non-isothermal solidification condition

Solid solution strengthening is essentially activated in Nickel-based superalloys, which means, the precipitation of coherent phases of Nb, Mo, Al, Ti or Ta phases in γ matrix. These precipitates can include γ' ($\text{Ni}_3(\text{Al, Ti, Nb})$) or BCT γ'' (Ni_3Nb) [50], generally formed during ageing. However, these alloys are prone to have Laves and/or δ during fabrication, the formation of the former precipitation is typical and independent of the alloy type; the latter one has been highlighted in 718 alloy fabricated by additive manufacturing process [155,156]. The formation of orthorhombic D0a Ni_3Nb δ -phase, transformed from the dissolution of Laves in the matrix [157], that can precipitate at grain boundaries and in grains as well [158], severely deteriorates the mechanical performance of the alloy. Therefore, any thermal treatments should avoid the precipitation of this needle-like morphology. One study revealed that the formation of this phase was mitigated by decreasing the stress-relieving temperature to 800 °C for one hour [159]. Formation of Nb-rich carbides and γ'' , the former type in micro scales and the latter in ultrafine size range, were reported during deposition by DED process [160]. Nevertheless, some experiments revealed that the γ'' precipitates during ageing process at a temperature range of 550 °C to 750 °C and the δ forms at 650 °C to 900 °C. Secondary carbides form in the expense of γ'' dissolution and dissolves at high ageing temperatures [161]. Some authors mentioned the occurrence of heat accumulation during fabrication of layers in favor of second phases formed in consequent layers as the result of an in situ heat treatment [156]. Thus, this study aimed to evaluate the effect of heat accumulation, during fabrication, on the microstructure, phase formation and the hardness of the Inconel 625 alloy deposited through DED. Regarding the numerical study, the material is simplified by focusing on selected phases and applying a surrogate approximate composition using a pseudo-ternary Ni-Al-Nb system [63]. Using ThermoCalc software and the Ni-Al-Nb pseudo-ternary database from Calphad gives the temperature-dependent equilibrium phase fractions, including $f^\delta(T)$, and $f^{\gamma''}(T)$, as the key factors in the precipitation as inputs in the prescribed formulation in the Chapter 4. In Table 7, the aforementioned parameters for the reaction rate calculation, interfacial and kinetic properties are summarized.

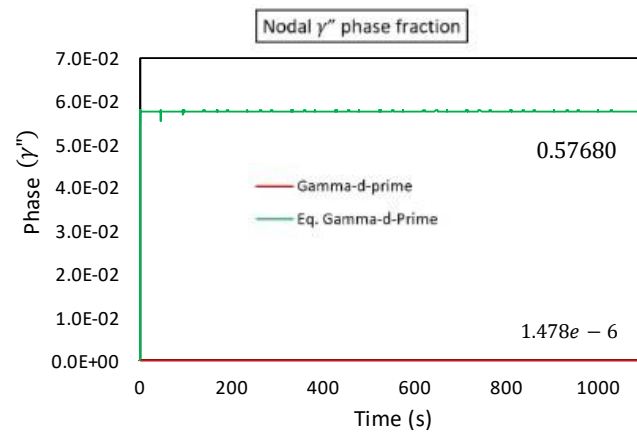
Table 7 List of symbols in reaction rate calculations and their values [162] [163]

Parameters	Description	Expression
α	Lattice constant of the matrix phase (β)	3.6 Å for γ matrix in In625
k_B	Boltzmann constant	$1.38 \times 10^{-23} \text{ J/K}$
γ_s	Interfacial energy between the matrix (β) and the precipitate (α)	0.105 J/m ² between γ and γ'' 1.000 J/m ² between γ and δ 0.151 J/m ² between γ and σ
V_m	Molar volume of the matrix phase (β)	$1.07 \times 10^{-5} \text{ m}^3/\text{mol}$ for γ matrix in In625
N_A	Avogadro constant	$6.022 \times 10^{23} \text{ mol}^{-1}$

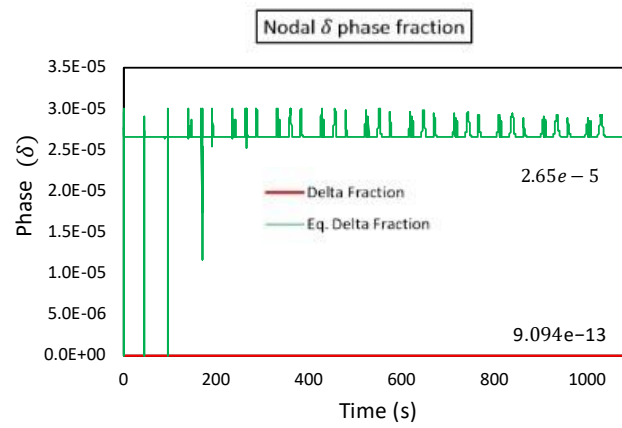
D	Diffusion coefficient	$8.8 \times 10^{-5} \text{m}^2/\text{s}$
ΔG_v	Bulk thermodynamic driving force for nucleation of the precipitate (α) in matrix phase (β)	$-0.46 \times (T - 700) \left(\frac{\text{J}}{\text{m}^3}\right) \gamma \rightarrow \gamma''$; $-0.8 \times (T - 700) - 1300 \left(\frac{\text{J}}{\text{m}^3}\right) \gamma \rightarrow \delta$;

In this section, relying on the predicted thermal history and calculated precipitate reaction rates as inputs, the non-isothermal JMA model is implemented into MATLAB scripts to acquire the phase fraction evolution at representative FE nodes. Incorporating all the chemical components and phases present in Inconel 625 in our framework is a numerically challenging task. Therefore, it is here simplified by focusing on selected phases and applying a surrogate approximate composition using a pseudo-ternary Ni-Al-Nb system [109]. Unlike γ'' which forms inside the grains through homogeneous nucleation, δ typically forms heterogeneously near the grain boundaries, but for simplifications, we just calculated the bulk case (inside the grains) and ignored the grain boundary conditions. In our simulations, we consider both thermodynamic equilibrium data and kinetic parameters to formulate the reaction rate constant, specifically the Avrami exponent (n). Detailed information about these kinetic parameters can be found in section 4.8.2. During the cooling process, the nucleation of precipitates follows the classical nucleation theory, and their growth mechanism is based on the 3D diffusion-controlled growth of spherical particles, as described in section 4.8.2. On the other hand, for the heating part of the graphs, we do not have thermodynamic and kinetic data for the reaction. Instead, we fit and estimate the dissolution factor using a simple power law equation, as $k_d = \alpha T^\beta$, where both α and β are approximated. This approach is based on the hypothesis that the growth and dissolution processes have different shapes and magnitudes. In Figures 63 (a-c) and 64 (a-c), we illustrate the phase precipitation versus the time of fabrication for points *A* and *B*, respectively. Due to the extremely fast cooling rate near the peak, the points of interest only experience a short period within the kinetically favorable temperature range. Consequently, only a small amount of precipitation forms during that time. As a result, the resulting precipitation phase fractions are relatively small, and the reaction becomes limited as the deposition continues. For example, in Figure 63 (a-b), point *A* the final fraction for γ'' , δ are (1.478e-6) and (9.094e-13) respectively. Additionally, point *B* exhibits a wider temperature range at the peak and a lower cooling rate compared to point *A*. This is attributed to the higher heat accumulation in the printed wall during fabrication, which is influenced by the melt pool size and multiple cycles of melting, as discussed in section 6.1.4.3. Figure 64 (a-b) presents the phase fractions for this point, where the values for phases γ'' , δ are (1.461e-6), and (3.23e-14) respectively. These values are 0.98, and 3.5 times smaller than those in node *A*. The 3D graphs depicted in Figure 64 (a-b) and Figure 66 (a-b) illustrate the phase fractions in time-temperature coordinates during the printing process for points *A* and *B*, respectively. These graphs demonstrate the exponential growth phase rate, represented by the red

dashed lines, indicating the growth of the phases as particles with a sigmoid behavior. By comparing the results in Figure 63 with Figure 65, it can be observed that the sigmoid graphs in point A indicate an extended diffusion time for nuclei and less time for growth, resulting in a larger number of nuclei but in smaller sizes. This observation aligns with the findings presented in [164], which highlight that the solvus temperature of γ'' , δ is below the solidus temperature of the γ matrix. Therefore, the formation of other phases during the additive manufacturing (AM) process would lead to an inhomogeneous composition distribution and varying initial composition within different positions of the entire AM build, affecting the precipitation [104]. Besides, it is documented in [164] that the strength of the additively manufactured parts is significantly lower than produced material with the conventional approach due to low precipitations of strengthening phases in AM parts, and it is suggested that ageing heat treatment is needed to exploit the maximum strength capabilities of Inconel 625. So, the proposed framework can be applicable to steer the deposition process to achieve the desirable volume fraction of secondary phases by adjusting pre-heating or setting the interlayer Dwell time to keep part in a favorable precipitation temperature range. Finally, it should be noted that other phases like Laves, and carbides may form during final stage of solidification in the complex precipitation system in AM process for multi-component and multi-phases Inconel 625. Understanding the evolution kinetics of all these phases would require reliable thermodynamic and interfacial energy databases.



(a)



(b)

Figure 63 Predicted phase fraction evolution for (a): γ'' , (b): δ for point of interest A vs time upon printing and solidification.

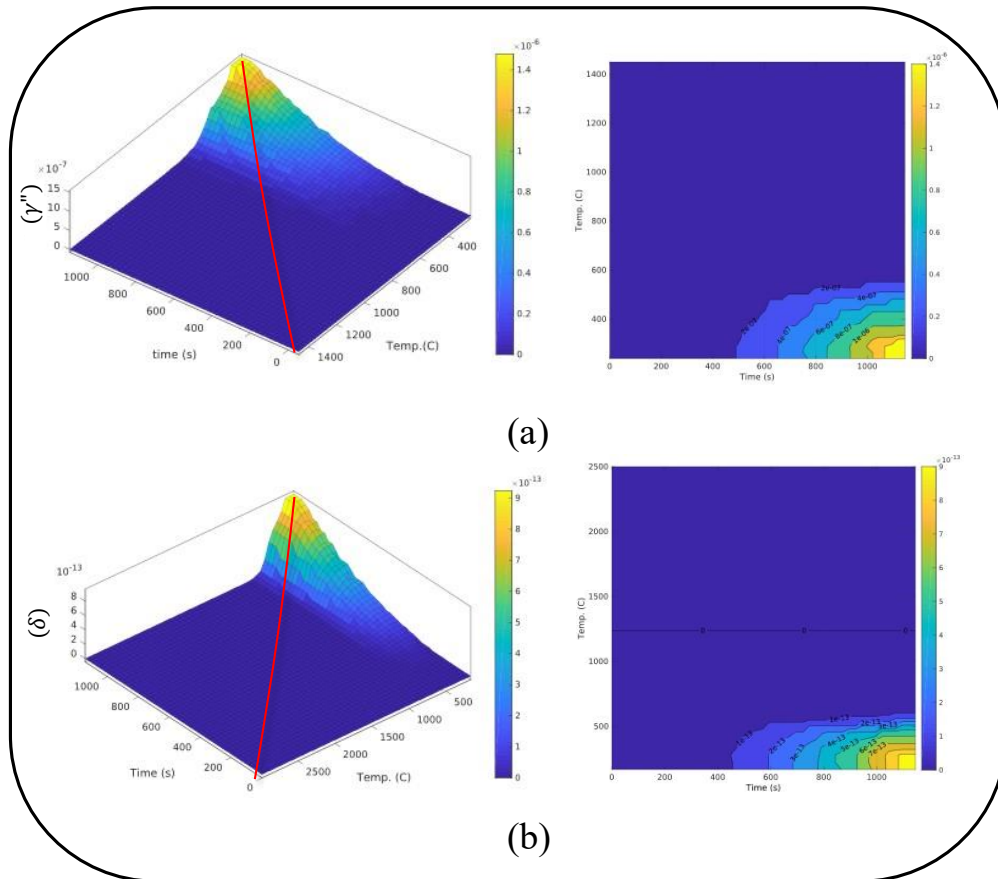
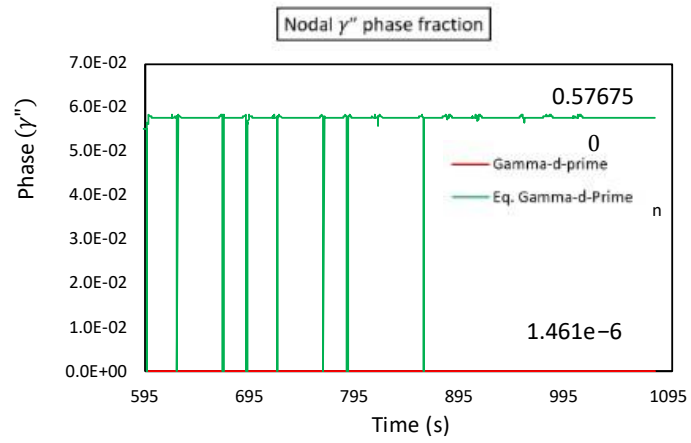
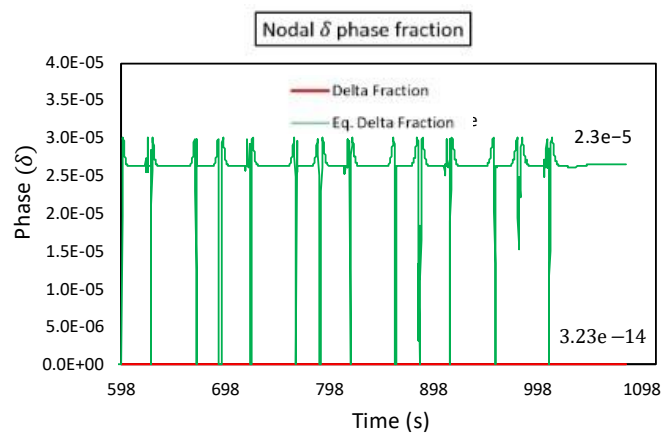


Figure 64 Predicted growing of the phase evolution for (a): γ'' , (b): δ in point of interest A.



(a)



(b)

Figure 65 Predicted phase fraction evolution for (a): γ'' , (b): δ for point of interest B vs time upon printing and solidification.

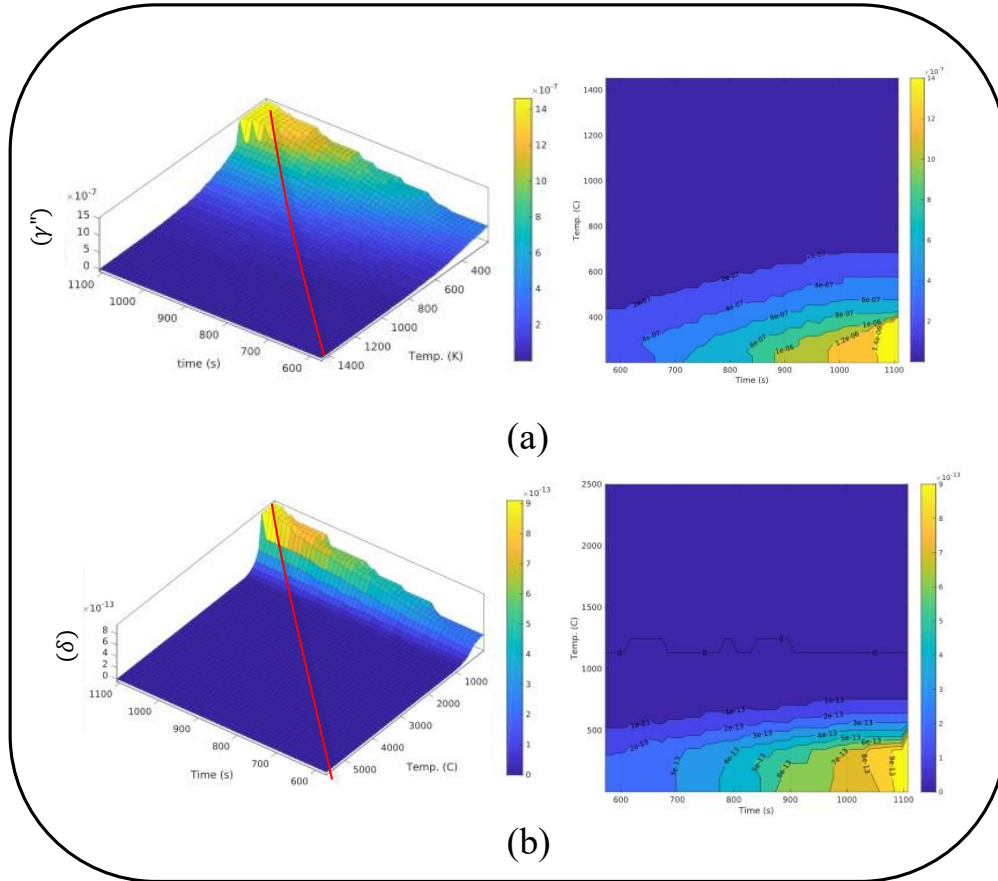


Figure 66 Predicted growing of the phase evolution for (a): γ'' , (b): δ in point of interest B.

Microstructural observations of the *C* and *D* regions, performed by SEM technique, do not confirm the presence of any carbide formation, as seen in Figure 67; however, the formation of oxides, independent of the position, and Laves phases is confirmed. It appears that the size and the concentration of the secondary phases, precipitated in the interdendritic spaces, such as laves have been affected by the location in the deposition height (bottom and top). As observed in Figure 67, Laves seem with larger size and smaller concentration on the topmost region. This can be justified by the heat accumulation of solidification rate, i.e., the increase in temperature and in solidification rate at the topmost region favours a larger diffusion of Nb and Mo in the γ matrix and, thus, a smaller nucleation occurs on the topmost region (as explained in Figures. 64 and 66). Regarding the size of precipitations, it can be attributed to the cycles of heating due to subsequent printing, meaning that laves phases were partially dissolved in the matrix, in the bottom region, whereas the precipitated Laves at the topmost region faced a larger growth time.

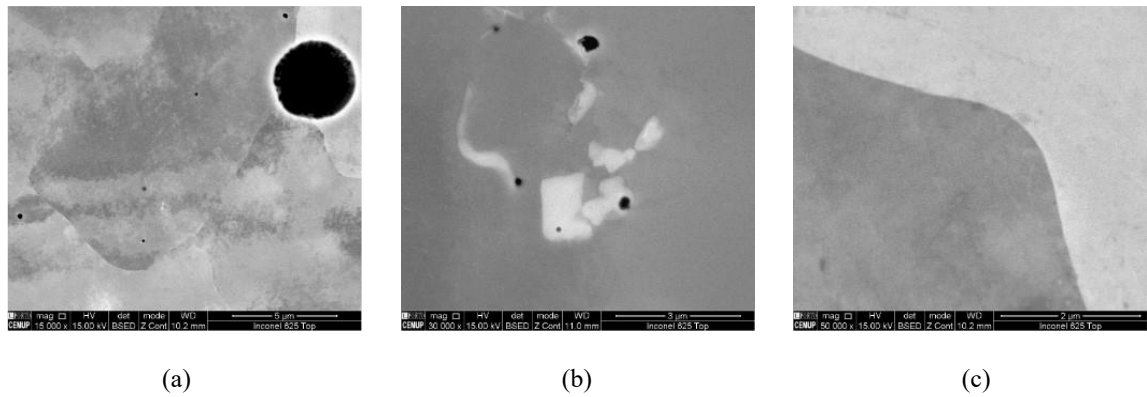


Figure 67 SEM electron backscattered images revealing (a): an oxide particle (mainly aluminum oxide) , (b): laves as bright regions and oxides as dark spots, (c): a clean grain boundary.

Subsequently, it is expected that the topmost region with larger grain size and low concentration of precipitations could have a smaller hardness. Thus, the hardness of similar specimens was measured by micro indentations. This analysis confirms that the bottom region (*C*) has a hardness of 257 ± 3 HV0.3 and the topmost region (*D*) has 238 ± 7 HV0.3.

6.1.4.5. Phase evolution with phase field method

In AM, the process involves multiple rapid heating and cooling cycles. These cycles can result in a more complex evolution of precipitates compared to a continuous cooling case, as both nucleation, growth, and dissolution, can occur concurrently during the process. The AM process can introduce a variety of challenges for predicting and controlling the evolution of precipitates. For example, the rapid heating and cooling cycles can result in uneven thermal gradients and thermal histories within the material, which can lead to a non-uniform precipitation behavior. Additionally, the presence of defects and residual stresses in the material resulting from the AM process can affect the distribution and morphology of the precipitates. Advanced modeling and simulation techniques, such as the phase-field method, can be used to understand and predict the evolution of the precipitates during AM. The phase-field method allows for the simulation of microstructure evolution over long time scales and can incorporate the effects of multiple precipitate species and other factors such as thermal gradients and diffusion anisotropy. This method can also capture the complex morphologies of precipitates that are difficult to describe using other models. To show the model capability in prediction of precipitation sizes and variants regarding to directions, the simulation results are compared with provided experiments from [165]. Then, the physics-based phase-field method in MOOSE that has emerged as a promising tool for simulating the precipitation-hardening behavior of materials like Inconel 625 in the prior section, is expanded to the AM case for two points of interests to study the effect of the location in the nucleation and then the evolution of the phases.

6.1.4.5.1. Calibration benchmark

Inconel 625 is a nickel-based superalloy that is widely used in high-temperature applications such as aerospace, nuclear, and chemical industries. It is known for its excellent corrosion resistance, high strength, and good weldability. One of the key factors that contribute to its high strength is the precipitation-hardening effect, which results from the formation of fine, coherent precipitates within the microstructure during heat treatment. However, achieving the desired microstructure and properties for Inconel 625 through heat treatment is a complex process that requires careful control of several processing parameters, such as temperature, time, and cooling rate. Moreover, the microstructure evolution during heat treatment is a slow and complicated process that can take hundreds or even thousands of hours to complete. Figure 68, in the context of the article by [165] shows the evolution of γ'' precipitate morphology during isothermal aging at 650°C. The simulated microstructure and experimental TEM (transmission electron microscopy) image in Figure 69 show that the γ'' precipitates coalesced with each other along their edges, but not face-to-face. This coalescence resulted in the formation of anti-phase boundaries (APBs) between the precipitates. The APBs occur when the crystallographic orientation of the precipitates on either side of the boundary is rotated by 180° relative to each other. Overall, the simulation results demonstrate the effectiveness of the phase-field method in capturing the complex evolution of precipitates during isothermal ageing. The morphological evolution of γ'' in Inconel 625, with its disk-shaped morphology and formation of antiphase boundaries, is consistent with previous experimental observations. Moreover, the simulated and experimental results showed that γ'' precipitates did not merge by coming face-to-face with each other during coarsening. Instead, the precipitates coalesced along their edges to form a disk-shaped morphology, leaving antiphase boundaries between them.

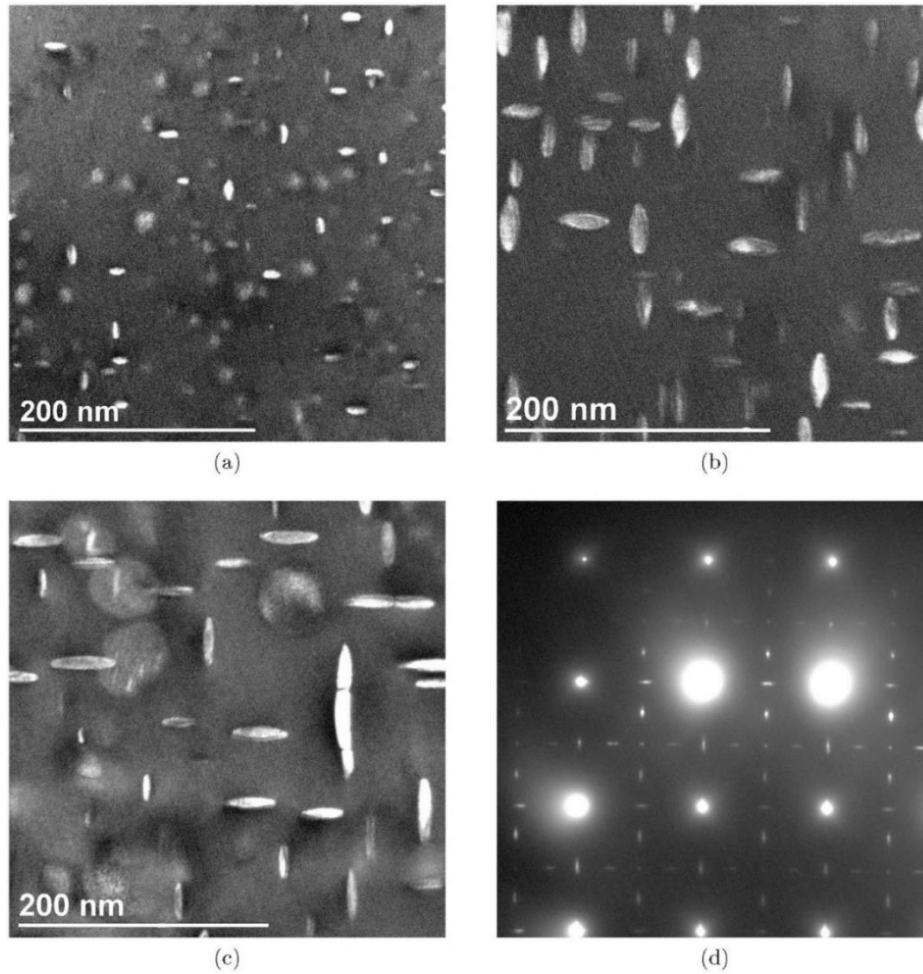


Figure 68 [001]-orientated dark field TEM images of γ'' precipitates in material aged at 650 °C for a: 100, b: 200 and c: 1000 h d: [001] selected area diffraction pattern [165].

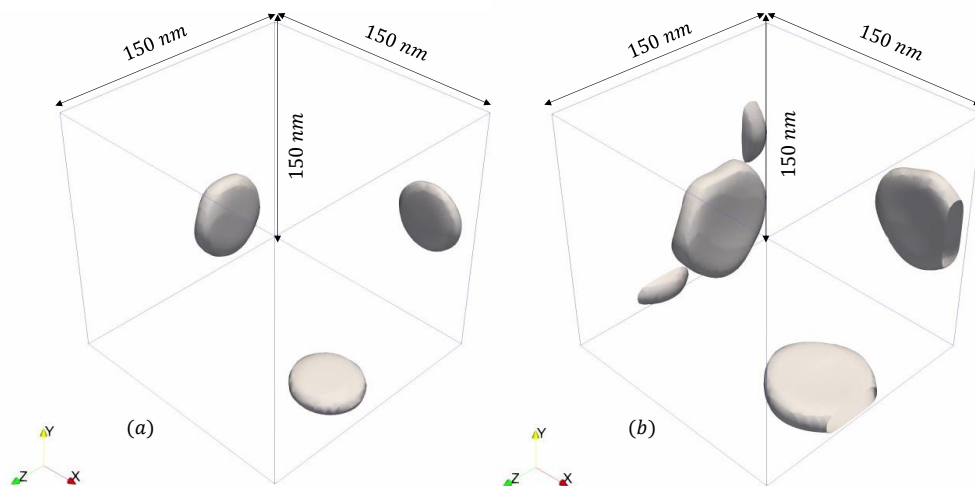


Figure 69 Phase-field simulation for microstructure of γ'' precipitates with three different variants in Inconel 625 aged at 650 °C for (a): 650 h, (b):1000 h for an RVE.

Taking advantage of the provided research results in [165] It appears that the mathematical relationship between ageing time (for 650 °C) and aspect ratio of precipitations is a hyperbolic decay relationship. The accuracy of our model is determined by comparing the experimental data fit with the average model data points shown in Figure 70 (a-c). The model is found to correctly reproduce the calibration data, with an almost perfect agreement with the experimental data fit achieved. Figure 70 (a-c) describes the evolution of mean particle length, aspect ratio, and volume fraction as calculated through phase-field simulations at 600 °C. The data was collected from three simulations with varying random seeds, and the mean particle length, aspect ratio, and volume fraction were calculated based on all the particles in the simulations. The simulated precipitate length and aspect ratio agreed with experimental measurements [165], but discrepancies occurred during early ageing stages, potentially due to the large critical nuclei size imposed on the nucleating particles. In the simulation, it can be observed that the anisotropic misfit strain tensor between γ'' precipitates and the γ matrix causes faster growth along the major axis than the minor axis. This led to a decrease in the aspect ratio (thickness/length) at a faster rate during early growth stages compared to later growth stages. The proposed phase-field model in this study assumes an isotropic interfacial energy and kinetics, which results in favorable agreement with experimental morphological data adopted from [165]. However, it is important to consider that the interface between tetragonal and cubic structures may exhibit strong anisotropic properties that could be incorporated into the model to improve its accuracy. Unfortunately, there is currently no information available on the magnitudes of such anisotropies for the γ/γ'' interface in the literatures. Hence, the study assumes isotropic interfacial properties due to the lack of relevant data. During the early aging stages, the volume fraction increases monotonically. This is primarily attributed to the free diffusional growth of the nucleated γ'' precipitates within the supersaturated γ matrix. However, the volume fraction eventually reaches a saturation level as the matrix's supersaturation level decreases and elastic interaction effects come into play. It should be mentioned that, the thermodynamic calculations report results as time approaches infinity, which is not feasible in practical applications.

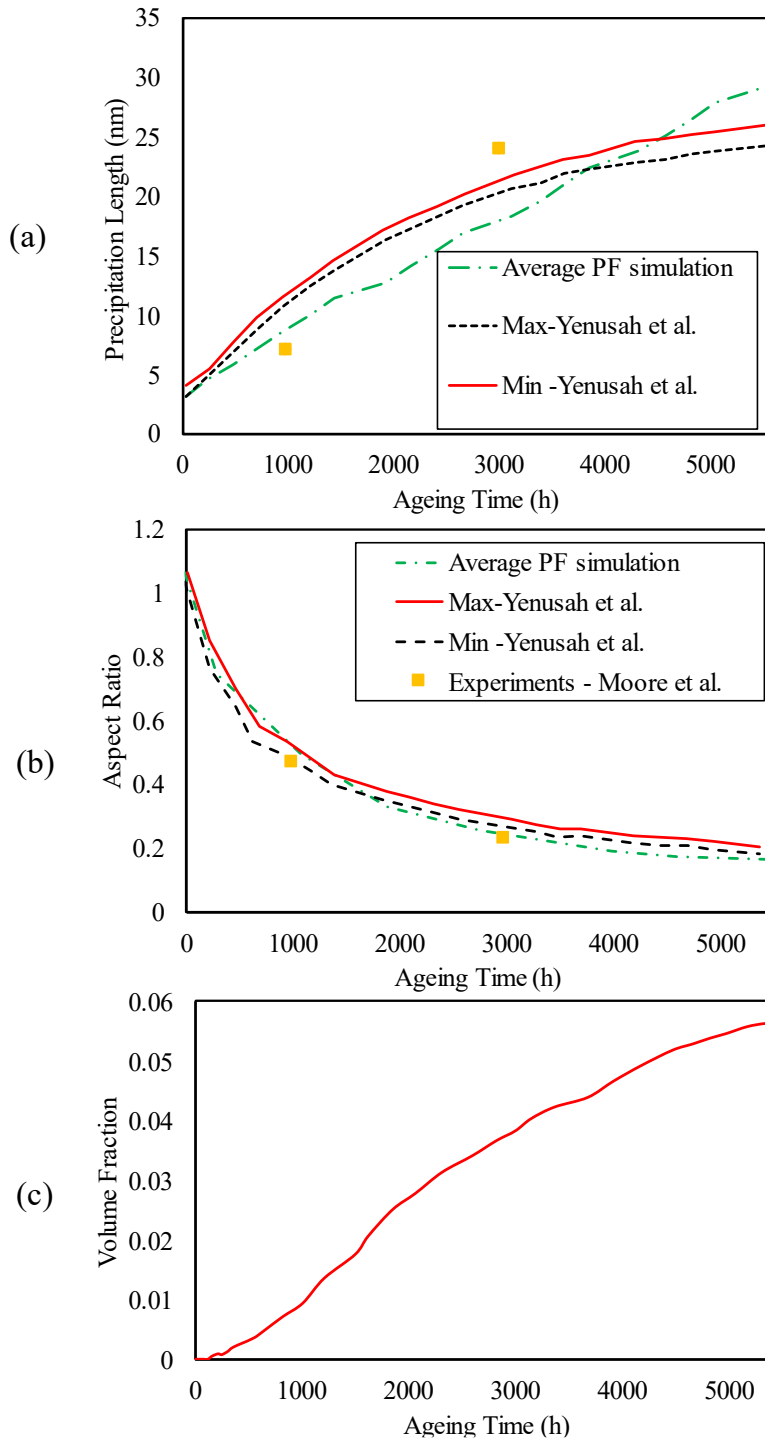


Figure 70 Simulated γ'' precipitation kinetics with PF in Inconel 625 aged at 600 °C and comparison with simulated results from [162] and experimental measurements [165]. (a) Precipitate length, (b) the precipitations aspect ratio, (c) volume fraction.

6.1.4.5.2. Phase-field simulations: γ'' evolution and kinetics

Figure 71 (a-e) illustrates the growth of precipitation in the lattice matrix locally and the elements' composition distribution across a line to emphasize how it varies during evolution. In the phase field model, the evolution of the system is governed by a set of partial differential equations that

describes the progress of a scalar field, which represents the order parameter distinguishing the different phases in the system (Figure 71 (a)). When γ'' starts precipitating, it creates regions of increased stiffness within the material, which can cause a local increase in elastic energy (see Figure 71 (a-b)). This is because the increased stiffness of the precipitate regions can lead to the creation of internal stresses as the material tries to maintain its overall shape. However, the formation of the precipitates can also reduce the overall elastic energy of the material. This is because the precipitates can act as barriers to dislocation motion, which can reduce the material's overall deformation energy. Additionally, the precipitates can create regions of reduced stress concentration, which can also reduce the overall elastic energy of the material. As the precipitate starts to form, the free energy of the system will increase due to the creation of an interface between the matrix and the precipitate. As the precipitate continues to grow, the free energy of the system will increase further due to the creation of additional interfaces between the matrix and the precipitate. However, the increase in energy may not be uniform throughout the system, as the formation and growth of the precipitate can create local variations in the energy. The local free energy term is the combination of the interfacial and chemical energy terms, when a precipitate is growing, between the matrix and precipitation, barrier functions increases and as much as interface gets smaller (like sharp interface model) in diffusive interface medium, the barrier function increases. In Figure 71 (c), near the double well potential function has two double edges that stems from interface; in real world it creates a barrier to the motion of defects such as dislocations and voids which can lead to an accumulation of stress and strain near the precipitate. The lattice displacement near a growing precipitate depends on several factors such as the composition and size of the precipitate, the nature of the interface between the precipitate and the matrix, and the thermal and mechanical history of the material. As a precipitate grows, it causes a lattice strain field in the matrix surrounding it. This lattice strain field arises (Figure 71 (d)) because the crystal structure of the precipitate may be different from that of the matrix, resulting in a lattice mismatch at the interface. The lattice mismatch can cause atoms in the matrix to move to accommodate the growing precipitate, leading to a local lattice distortion. The precise chemical distribution of the elements around the γ'' precipitate will depend on various factors, such as the initial composition of the alloy, the temperature and time of the precipitation process, and the nature of the interface between the γ'' precipitate and the matrix. The diffusion of Al into the γ'' precipitate is typically faster than the diffusion of Nb and Ni. Therefore, as the precipitate grows, it can become increasingly enriched in Al, while the surrounding matrix becomes relatively depleted in these elements. At the same time, the concentration of Nb and Ni in the matrix near the precipitate can increase and decrease respectively (Nb precipitate slower due to its slower diffusion rates). Inside the γ'' precipitates, the Nb and Al atoms can occupy different crystallographic sites, depending on their size and charge. Typically, Nb atoms prefer to occupy the octahedral sites in the γ'' lattice, while Al atoms prefer the tetrahedral sites. The distribution

of Nb and Al atoms within the γ'' precipitate can affect its properties, such as its lattice parameter, elastic modulus, and hardness.

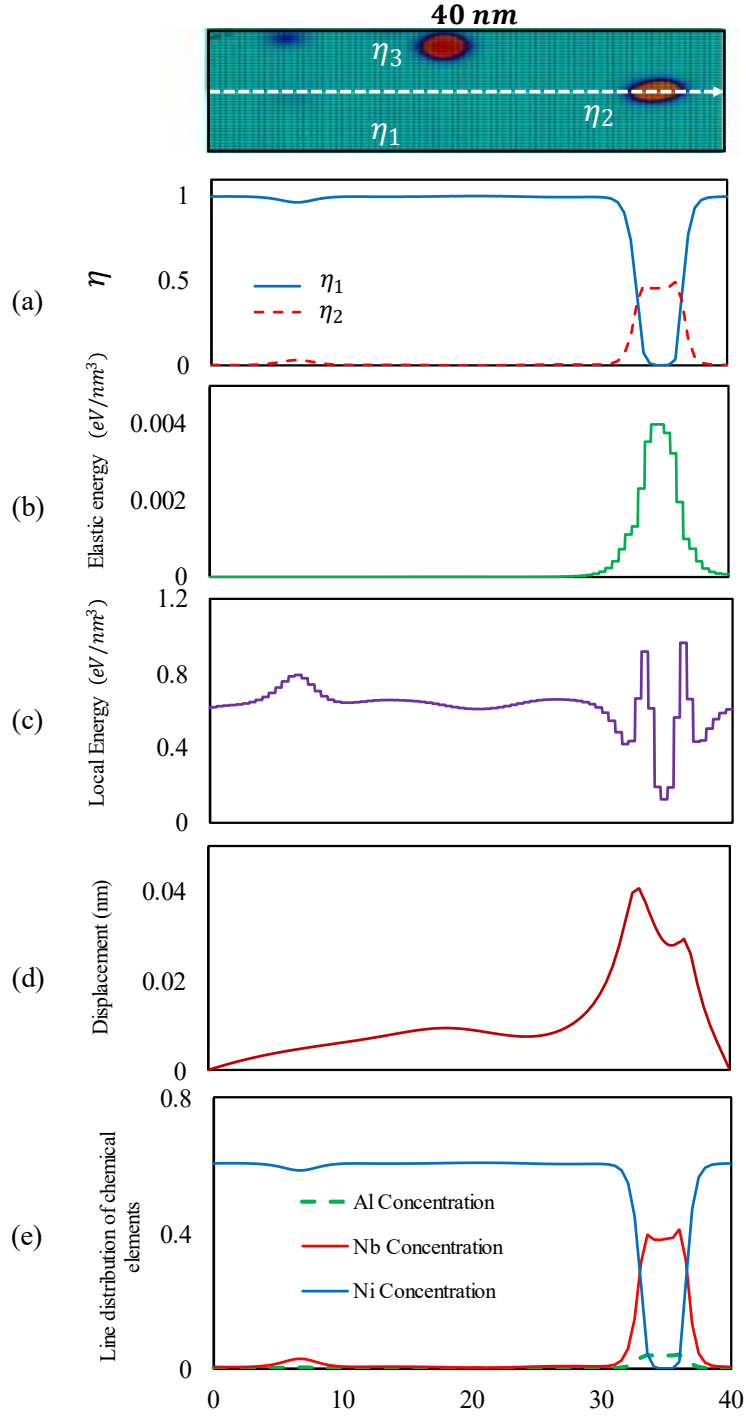


Figure 71 (a) non-conserved order parameter representative of the phase growing, (b) Elastic energy of lattice during precipitation evolution, (c) Local energy term variation due to the precipitation growing, (d) lattice displacement induced by misfit phenomena, (e) Ni, Nb, Al concentration varies along line.

6.1.4.5.3. Precipitate evolution under a complex thermal history: rapid thermal cycling

In this stage, the temperature evolution for two points of interest are imported to the precipitation phase field coding to evaluate the effect of the various temporal oscillations in DED process. Herein, we mimicked the experimental effort with inspiration from Denlinger et al. [166,167] as shown in Figure 72. During the process of building a component, each location experiences multiple rapid cycles of heating and cooling, which can be seen in Figure 73.

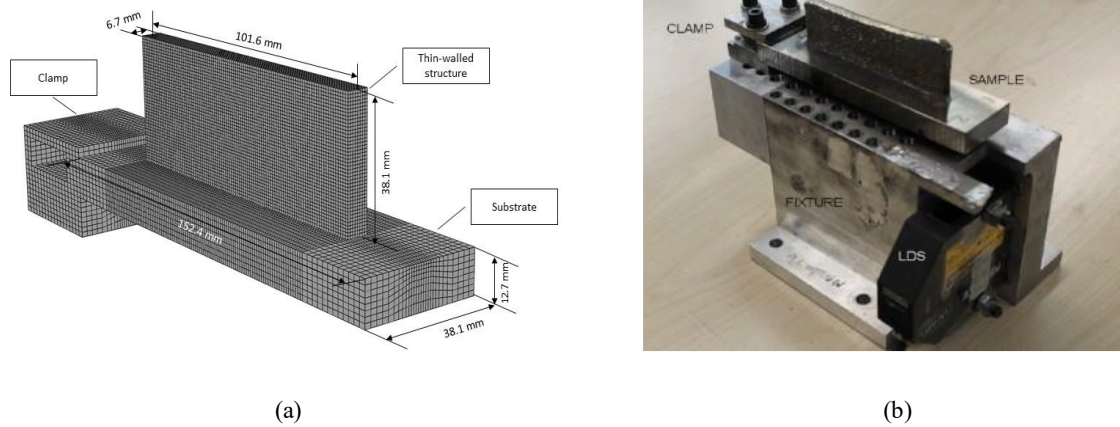


Figure 72 (a) The utilized finite element meshes for assembly, (b) experimental set-up adapted from [166,167]

In the fabricated thin-walled part, two nodes are selected as the points of interest and labeled as A and B to study the temperature evolution (see Figure 73 (a)) and phase fraction analysis. Nodal graph of temperature in aforementioned points are down in Figure 73 (b, c) to be used for the next sections.

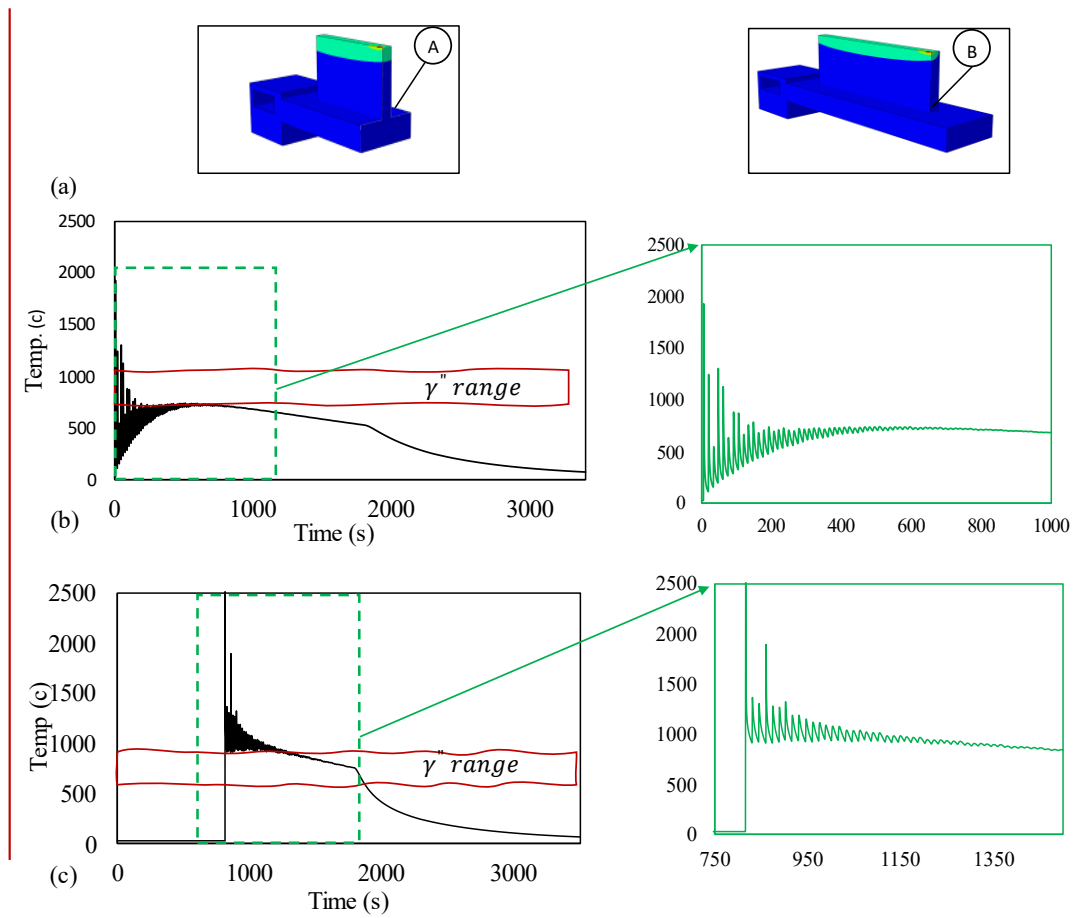


Figure 73 Transient temperature map for printed part with two sections contains A and B, (b): Temperature evolution vs time for point A, (c): Temperature evolution vs time for point B.

This causes the temperature at a given location to cross the threshold for γ'' formation multiple times. Additionally, the thermal history of different regions of the component may be different, and this can be controlled by the underlying process parameters. Therefore, it is important to understand how the growth of precipitates may vary at different locations in the component and how it can be influenced by the process parameters. Understanding the role of process parameters is crucial for developing new printing strategies that can lead to parts with superior mechanical properties. To simulate the formation of precipitates for the cantilever introduced in Chapter 4, we will use phase field simulations along with the part-scale thermal model in this section. In the points called A and B the highest cooling rate ranges are 1396 °C/s and 1383 °C/s respectively.

For the Representative Volume Elements (RVEs), the presence of grain boundaries is considered in the evolution of the phase fraction. As demonstrated by Laskowski et al. in [168], lower cooling rates and even continuous cooling transformation (CCT) conditions do not result in precipitation. However, they found that applying fictive oscillations with varying cooling rates and periods leads to significant changes in the precipitated particles, and at the highest cooling rate, precipitation may occur. Our current case study aligns with these findings, indicating that the precipitated particles in the RVEs are strongly influenced by the thermal cycles and oscillations actively applied during the simulation. Despite the fast heating and cooling rates, the repeated exposure of the system to a specific temperature range appears to be the dominant factor influencing its behavior. By comparing points A and B (Figures 74 (a-d) and Figure 75 (a-d)), we observe that A, with a higher range of thermal cycling and a more uniform pattern, initially has fewer nuclei compared to B. However, as the number of cooling and heating cycles increases, it may lead to the formation of a higher number of nuclei, reaching the critical volume required for nucleation. This may result in the formation of more stable nuclei that do not dissolve during subsequent thermal cycling, leading to a higher degree of precipitation and altered material properties. It can be stated that fluctuations in thermal cycling may speed up the precipitation process. This is because rapid cooling rates can increase the undercooling of the matrix material, which can promote the nucleation and growth of γ'' precipitates. Additionally, faster cooling rates can also suppress the diffusion of solute atoms within the matrix material, which can enhance the stability of the γ'' precipitates. As Laskowski et al. in [168] explained, we confirmed that even at higher range of temperature, due to the short time span, the precipitations may not dissolve completely during heating up. Beyond 1112 s, the precipitations nucleation's is limited and precipitations experienced coarsening.

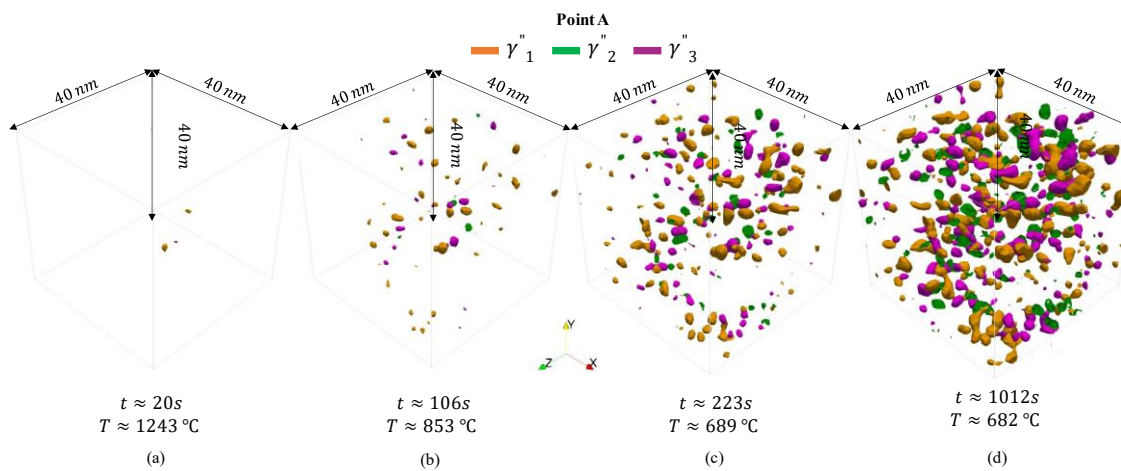


Figure 74 In-situ evolution of precipitations the laser fabrication process for point of interest A.

The provide evidence for point *B* shows the higher range of temperature and faster cooling rate leads to a greater number of nuclei at first cycle, with more similar rounded shape in comparison with irregular shape of nuclei in *A*. In point *B*, after 1516 s, the evolution of precipitations is limited by growing of nucleation and then undergoes coarsening. In this scenario, the accumulated heat in a structure at point *A* is greater than that at point *B* over longer periods of time, resulting in an increased number of precipitations overall. The overall volume fraction of γ'' precipitates measured around 0.0487 at 3670 s for point *A*, whereas it is approximately 0.0983 at the same time for point *B*.

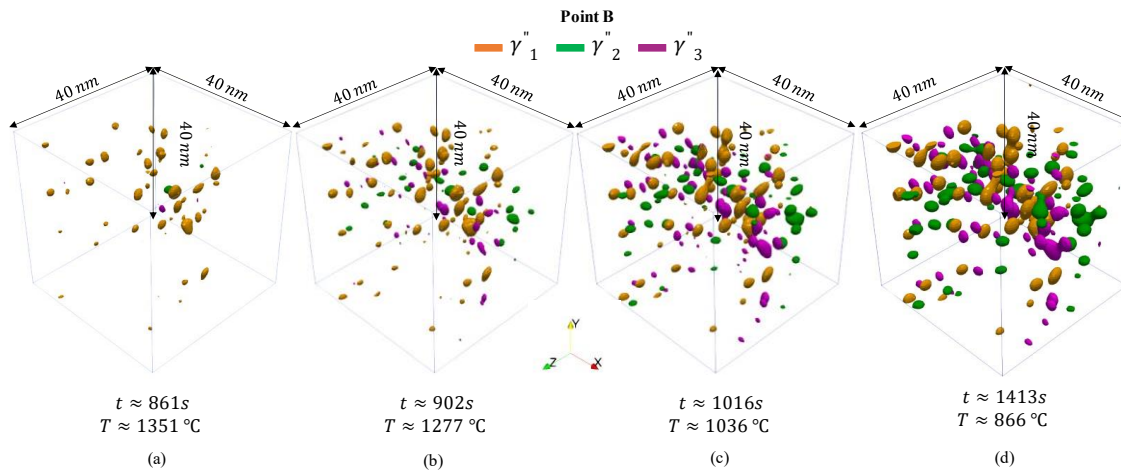


Figure 75 In-situ evolution of precipitations the laser fabrication process for point of interest *B*.

Due to the fast nature of the thermal cycles, it is challenging to directly examine the precipitate evolution in situ during experiments. Nevertheless, some attempts have been made to study the influence of such cycles on the precipitation process in certain materials. For instance, a recent study focused on the high CMSX-4 super-alloy [169], while to the best knowledge of the author, there is currently no experimental research on the effect of repetitive thermal cycles on the precipitation process in Inconel 625, which is a more complex alloy. In [170], the effect of a single hill shape of temperature oscillation is studied on creatures of the precipitations for Inconel 718. The effect of the Nb diffusion in precipitation size is shown in Figure 76, it can be seen that in the first variation of γ'' , there is a lower concentration in comparison with two other variations. Increasing locally the concentration of Nb in lattice structure can lead to a decrease in the size of the γ'' precipitates. This is because Nb can enhance the coherency between the precipitates and the matrix, which inhibits the growth of the γ'' precipitates. On the other hand, we found Al doesn't have significant effect in this trading off.

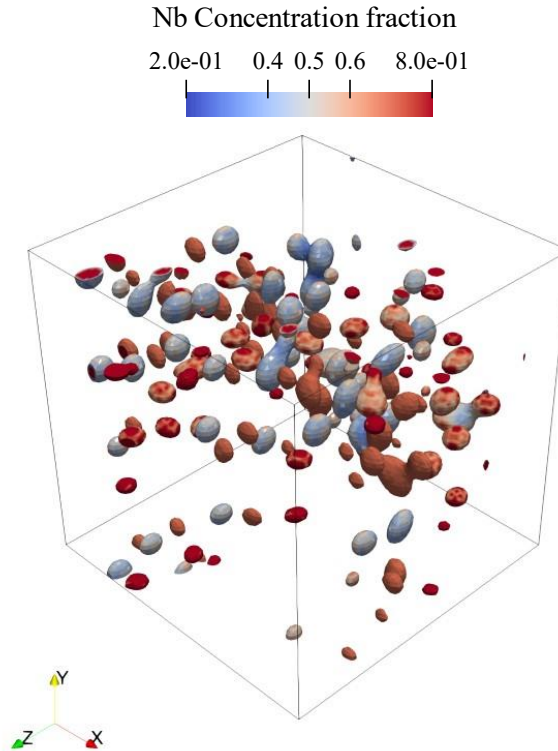


Figure 76 Fraction of Nb concentration in precipitation for point of interest B.

6.1.4.5.4. γ'' coherent strengthening

The precipitation hardening mechanism of Inconel 625 leads to an increase in yield strength as shown in Equation 6.8 for two points *A* and *B* as two RVEs (see Figure77). The dispersed γ'' precipitates act as obstacles to the movement of dislocations, impeding their motion and making it more difficult for the material to deform. As a result, the yield strength of the additive manufactured Inconel 625 parts is significantly enhanced, providing better resistance to plastic deformation and improved structural integrity.

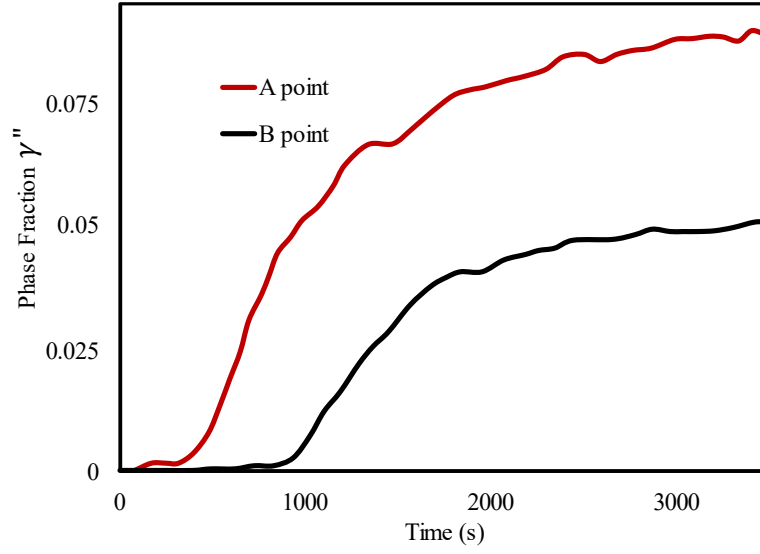


Figure 77 γ'' fraction evolution for points A and B.

$$\sigma_{coherency}(MPa) = 1.7MG|\epsilon|^{1.5}\left(\frac{h^{1.2}f(1-\beta)}{2bR}\right)^{0.5} \quad (6.8)$$

The Taylor factor, denoted by M , has a value of 3.06 for materials with a face-centered cubic (FCC) crystal structure. The shear modulus, represented by G , is equal to 56 GPa [171]. The tetragonal lattice misfit, denoted by ϵ , describes the mismatch between the lattice parameters of the precipitates and the surrounding matrix and is set to 0.0372 [172]. The equation also includes the volume fraction of precipitates, f . The average aspect ratio of the particles is denoted by R , while h represents the average length of the particles. Additionally, the equation incorporates the constant β , which takes the value of 1/3 when all three variants of precipitates are observed. Finally, the magnitude of Burger's vector, denoted by $b = 2.4$, refers to a specific crystallographic property associated with dislocations in the material. The corresponding parameters for the two points A and B , are provided in Table 8 and the derived value of coherency strength is depicted in Figure 78.

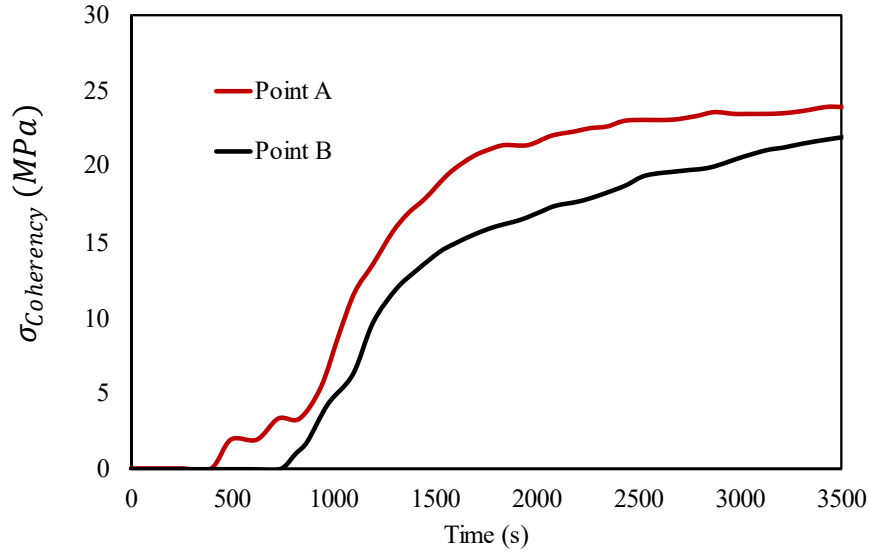


Figure 78 γ'' coherent strengthening for points A and B

Table 8 characterization of γ'' in Inconel 625 for two points A and B as two RVEs

PFM	Avg. h(nm)	Avg. R(nm)	f(-)	$\sigma_{coherency}(MPa)$
Point A	2.93	0.7	0.0481	23.92
Point B	4.02	0.9	0.0983	21.88

6.2. Fully Coupled PF model responses

In this section, we showcase and discuss the simulation results obtained from the proposed model, demonstrating its reliability in effectively coupling the temperature and phase field formulations with mechanical responses. Firstly, we evaluate its performance by employing benchmark melt pool geometries provided by NIST [173]. Subsequently, we analyze and discuss the computational results obtained from processing a single circular path. The simulations are performed on a computer cluster equipped with 2 Intel CPUs (16 cores total), and 128 GB of RAM. The CPU nodes are connected via a 40 Gbps InfiniBand network, which allows for efficient communication between the CPU nodes and enables the efficient use of parallel computing resources

6.2.1. Material State Variables in Allen-Cahn Phase Field Model

The phase-field parameters related to Inconel 625 are given in Table 9. The CALPHAD approach is widely used for the evaluation and compilation of the thermodynamic and kinetic input data in quantitative PF modeling of multi-physics systems. Direct incorporation of the CALPHAD

library into the MOOSE environment enables seamless access to extensive thermodynamic and kinetic databases, improving the accuracy and reliability of PF simulations [137]. In addition, the material properties associated with the temperature and phase parameters are listed in Tables 10 and 11. The parameter φ in Table 11 represents the consolidation, defined as a phase indicator value for tracking the powder transformation into the solidified state. This parameter is inherently irreversible, i.e., $\varphi = \max\{\phi(t), \phi(t + dt)\}$, taking the maximum value of $\phi(t)$ within two consecutive steps. This is consistent with the fact that the solidified material is in a lower energy state than the liquid or powder state, thus, it is thermodynamically unfavorable for the material to return to a higher energy state.

Table 9 Phase field parameters for Inconel 625 [140–142].

Parameters	Value	Units
Kinetic coefficient (μ_ϕ)	0.5	$mm\ K^{-1}s^{-1}$
Interface width (δ)	1	mm
Surface tension (ω)	65×10^{-6}	$mJ\ mm^{-2}$
Latent heat (L)	23.8×10^9	$mJ.tonne^{-2}$
Melting temperature (T_M)	1730	K

Table 10 Material properties as the function of the phase-field parameter [174].

Material properties	Equations	Molten phase	Solidified phase
Thermal conductivity (κ) (W/mmK)	$\kappa(\phi) = \phi \kappa_m + (1 - \phi) \kappa_d$	$\kappa_m = 30.25$	$\kappa_d = 11.10$
Specific heat capacity (c) (J/mm^3K)	$c(\phi) = \phi c_m + (1 - \phi) c_d$	$c_m = 5.06$	$c_d = 3.30$
Thermal expansion(ξ) ($1/K$)	$\xi(\phi) = \phi \xi_m + (1 - \phi) \xi_d$	$\xi_m = 15 \times 10^{-6}$	$\xi_d = 10 \times 10^{-6}$
Young's modulus (E) GPa	$E(\phi) = \phi E_m + (1 - \phi) E_d$	$E_m = 85$	$E_d = 210$
Yield Stress (σ_Y) GPa	$\sigma_Y(\phi) = \phi \sigma_{Ym} + (1 - \phi) \sigma_{Yd}$	$\sigma_{Ym} = 0.03$	$\sigma_{Yd} = 0.24$

Table 11 Material properties as the function of the consolidation parameter [24].

Material properties	Equations	Powder phase	Dense phase
Density (ρ) (kg/mm^3)	$\rho(\varphi) = (1 - \varphi) \rho_p + \varphi \rho_d$	$\rho_p = 4460$	$\rho_d = 7780$

6.2.2. Spatial and time discretization

The laser spot diameter used in this work is chosen significantly smaller than the size of the part, with a ratio ranging from 10 to over 10000. To ensure an accurate representation of the high thermal gradient and effective modeling of the heat flux in the heat-affected zone area, it is imperative to utilize a fine mesh structure around the laser spot. In Figure 79, the maximum temperature in the center of the melt pool is plotted against the variation in the mesh size, specifically after 0.25 ms. It is evident that, by utilizing higher mesh density, the maximum temperature reaches a plateau, indicating convergence in the

temperature distribution. This observation allows for a balanced approach, wherein the utilization of finer meshes accommodates both solution accuracy and the computational scale of the FE system. We note that the maximum temperature difference between refined elements, with sizes 0.0625 and 0.03125, is found to be less than 1%. This signifies the minimal impact of the chosen element sizes on the temperature distribution, further supporting the choice of the mesh refinement strategy in the present modeling framework. For the remaining part of the study, the subsequent element size in adaptive mesh refinement (AMR) in the upcoming sections is set to 0.0625 mm.

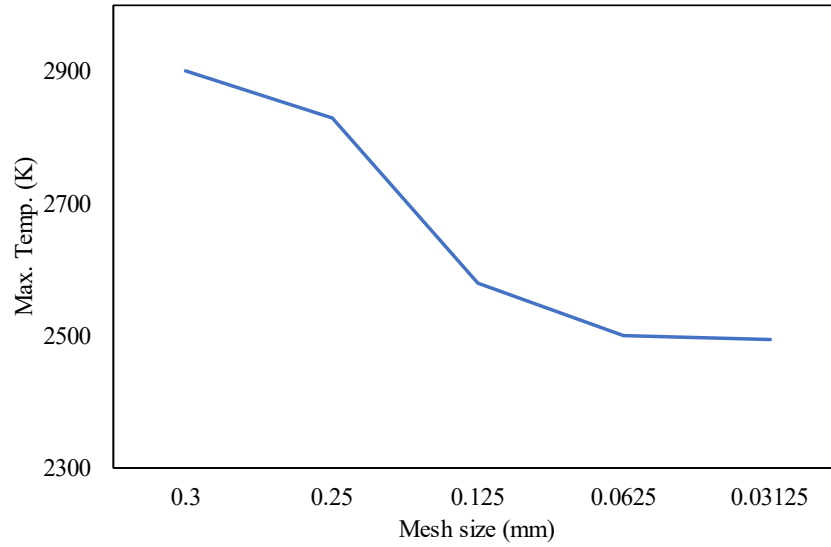


Figure 79 Comparison of temperature distribution in the center of melt pool for different mesh sizes.

In the current transient heat transfer scenario, with a heat source that undergoes motion at a known velocity, v , it is crucial to ensure a continuous distribution of the heat source across the simulation domain without skipping any elements. Thus, the maximum allowable time step, Δt , is determined by the relationship $\Delta t = d/v$, where d represents the diameter of the laser spot. This restriction prevents the heat source from bypassing elements as it progresses through the simulation domain.

6.2.3. Benchmark example

We start by investigating the benchmark tests following a standardized and well-defined set of experimental conditions provided by NIST, allowing for a direct comparison between the measured values and the results obtained from numerical process simulations. The simulation models were calibrated by adjusting various parameters and input values to closely match the experimental data. This calibration process aimed to improve the accuracy and reliability of the simulation results, ensuring the accurate representation of the physical phenomena occurring during the present additive manufacturing process. Nickel-based superalloy 625 (IN625) substrates with sizes 24.5 mm $\times$ 4.5 mm, and 3.2 mm thickness were selected, and the utilized powder in the benchmark is of the same material. One specific group of PBF experiments was selected for the rest of this study, which is the so-called “Additive

Manufacturing Metrology Testbed” (AMMT) [175]. For this experimental setting, the laser size had a 4-sigma diameter ($D4\sigma$) range equal to $170\ \mu\text{m}$ (full-width half max (FWHM) of $100\ \mu\text{m}$). The detailed information about the experimental setup can be found in [176] for interested readers. The Goldak's double-elliptical model was utilized for the heat source. The proposed numerical model described in previous section is simulated based on two scenarios: Case B with laser power $179.2\ \text{W}$ and scanning speed of $800\ \text{mm/s}$, and Case C with laser power $179.2\ \text{W}$ and scanning speed of $1200\ \text{mm/s}$. Figure 80 (a-d) illustrates the transparent view of the powder consolidation evolution for Case B with dimension $2000 \times 800 \times 200\ \mu\text{m}^3$ during four-time steps. The thickness of powder layer is considered $36\ \mu\text{m}$ according to Lane et al. [175].

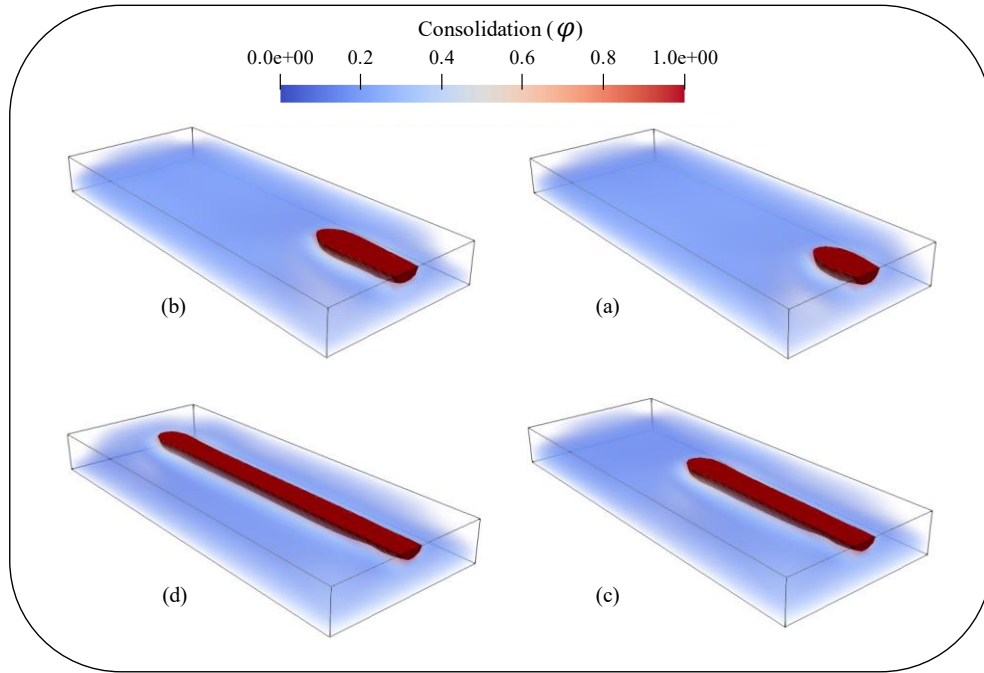


Figure 80 Transparent view of the consolidated powder after absorbing laser energy indicated by red colour, and the mushy region that shows interval of molten and unmelted powders on the substrate of size $10 \times 4 \times 1\ \text{mm}^3$ at four different time steps: (a) $t = 0.5\ \text{ms}$, (b) $t = 1.25\ \text{ms}$, (c) $t = 2.55\ \text{ms}$, and (d). $t = 4\ \text{ms}$.

Allied with the calibration objective, Figures 81 and 82 (a-c) showcase and analyze Cases B and C for AMMT to explore the characteristics of the melt pools. As indicated in Figures. 81 (d) and 82 (d), the corresponding samples were cross-sectioned through the center of the laser traces (across the line “A-A”). Subsequently, standard metallurgical sample preparation techniques were employed, including mounting and polishing, to facilitate a comparison with the overall shape of the modeled melt pools. This approach enables a qualitative assessment of the simulated melt pool's conformity with the actual physical samples obtained through cross-sectioning and sample preparation.

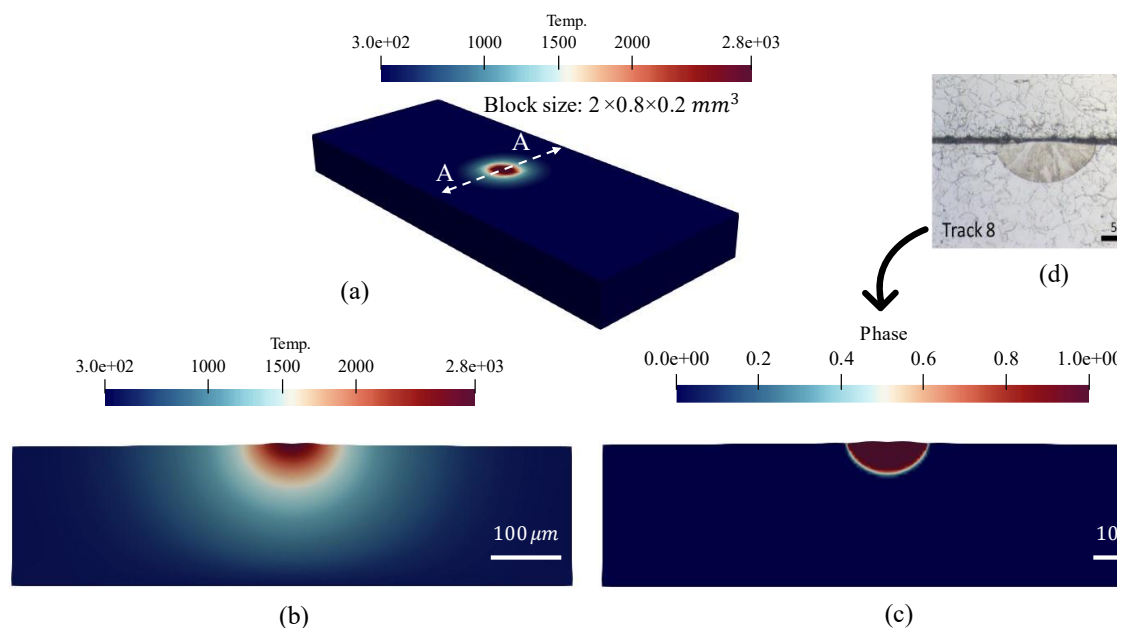


Figure 81 Simulation results of Case C: 179.2 W, 1200 mm/s (AMMT), (a) Temperature evolution in the center of trace, (b) Cross-sectional temperature alongside of line A-A, (c) phase field variable alongside of line A-A, (d) Experimental cross-sectional adapted from Heigel et al. [176].

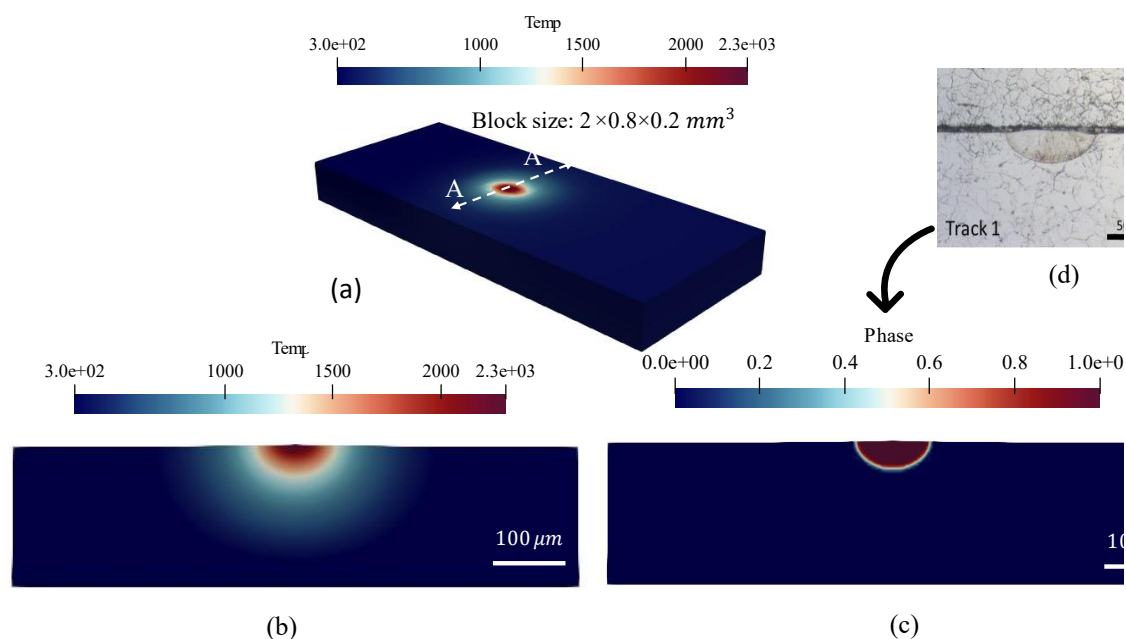


Figure 82 Simulation results of Case B: 179.2 W, 800 mm/s (AMMT), (a) Temperature evolution in the center of trace, (b) Cross-sectional temperature alongside of line A-A, (c) phase field variable alongside of line A-A, (d): Experimental cross-sectional adapted from Heigel et al. [176].

A close agreement between the simulation results and the experimental measurements taken from the AMMT samples [176] were found, as evidenced in Table 12.

Table 12 Comparison of the simulation and experimental benchmarked by NIST [175,176].

AMMT melt pool dimensions	Case C	Case B
Average width by NIST (μm)	106.02	123.46
Width by PF-AC (μm)	102.96	116.83
Average depth by NIST (μm)	29.15	35.96
Depth by PF-AC (μm)	39.61	45.53

6.2.4. Full circle path example

In this section, the previously developed formulation is applied to a 3D geometric case. The particular example being examined is a thin layer of powder, with an initial thickness of 0.2 mm , modeled on top of a substrate. The substrate has a volume of $10 \times 10 \times 2\text{ mm}^3$ and is made of the same material as the powder. A moving ellipsoidal heat flux was utilized to melt particles on the surface of the powder layer, as shown in Figure 83. The heat source setting is assumed as in the previous example and its associated parameters are listed in Table 13.

Table 13 Heat source parameters in 3D distribution.

Parameters	Value	Units
Laser power (P)	100	W
Efficiency (α)	0.60	—
Scalling factor (β)	2	—
Radius ($r_x r_y r_z$)	0.5	mm
Scanning speed (v_x, v_y, v_z)	2000	mm/s

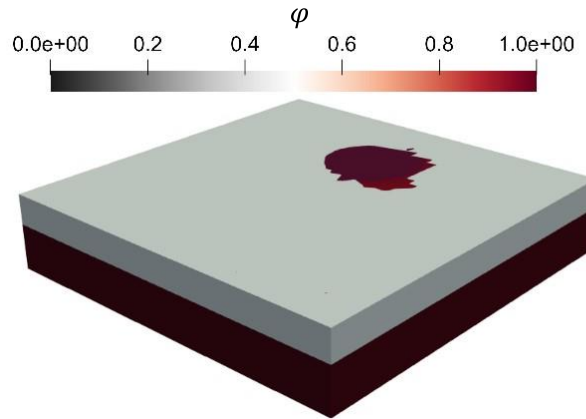


Figure 83 Consolidated powder layer on the top of substrate with a contour of the phase indicator.

Figure 84 illustrates the consolidated powder after laser processing on the top surface of the compacted powder layer. The phase indicator in the image is used to show the state of the material after solidification, from powder state ($\phi = 0$), to solidified state ($\phi = 1$), while the mushy area ($0 < \phi < 1$) representing the state between the powder and consolidated part (the transitioning white area around the molten region).

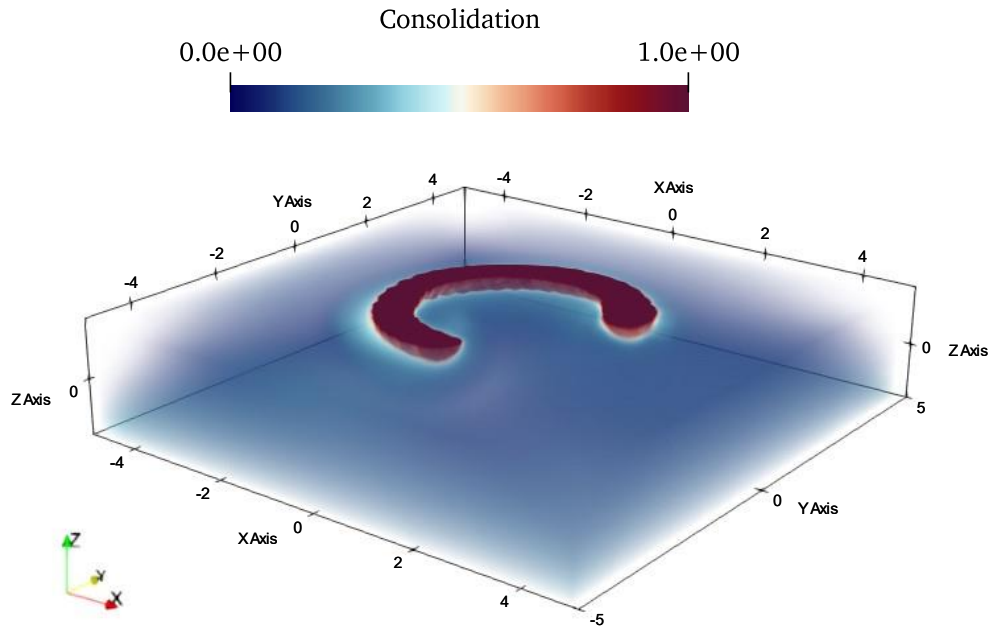


Figure 84 Transparent view of the consolidated powder after absorbing laser energy indicated by red colour and the mushy region that shows interval of molten and unmelted powders.

The variation of the phase field variable (ϕ) with temperature across the A-B line is illustrated in Figure 85 (a). In Figure 85 (b), the three-dimensional view of the free energy density term as the function of phase parameters in the spatial domain (x), which is mentioned in Figure 85 (a), is shown. The minimization of the homogeneous free energy density allows for determining the suitable thermomechanical properties for the particular domain in the system. Thus, the system will be able to respond dynamically to the changing conditions created by the laser melting and solidification process and enables modelling the powder phase changes.

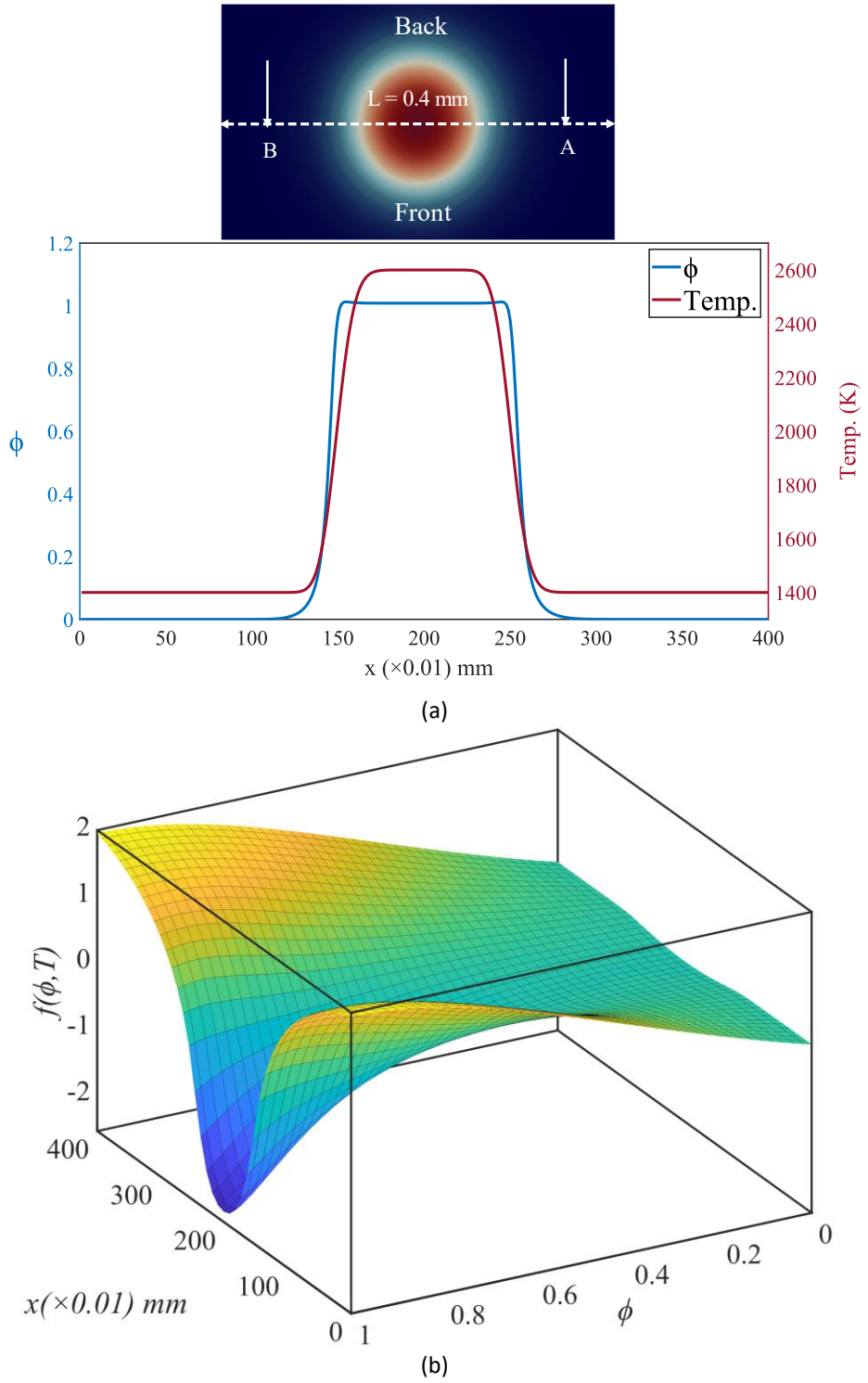
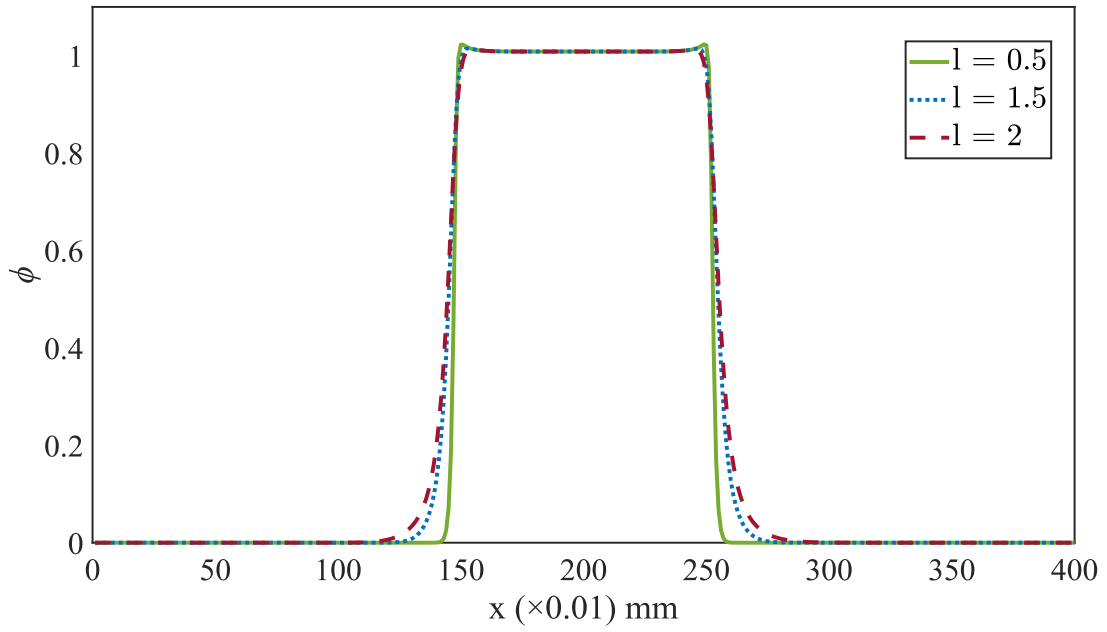


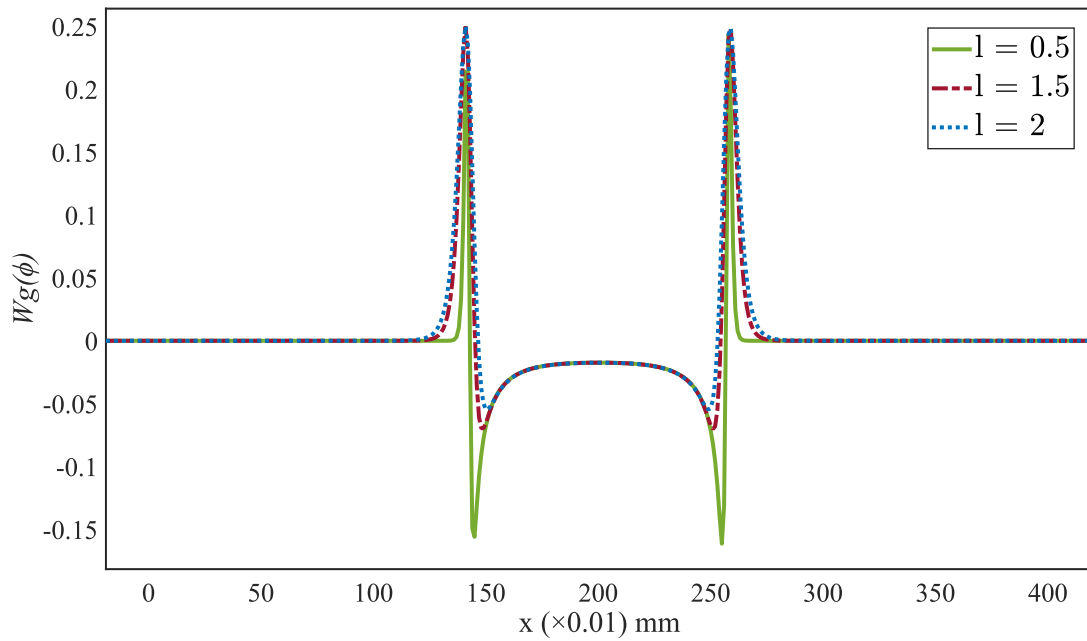
Figure 85 (a): Phase field graph vs temperature evolution in the domain of a melt pool boundary with $l = 2$ across A-B line, (b): 3D view of the changes of free energy density function with the phase-field in the spatial domain across A-B line.

Three different values of phase-field length scale (l) parameter were used to investigate its influence on both the temperature evolution in the transient solution and the phase-field variable (ϕ), as shown in Figure 86 (a). For the choice of $l = 0.5$ mm, lowest phase field diffusivity is observed and the system

exhibits behavior similar to the predictions of sharp interface theory. This choice results in a higher number of iterations required to capture the moving interface, which in turn leads to an increase in the variation of the barrier energy term describing the energy cost of transforming from one phase to another, as depicted in Figure 86 (b). The magnitude of the barrier energy term represents the energy cost of the phase transition and its shape represents the kinetics of the phase transition, with a narrower barrier indicating a faster transition. The impact of increase in the barrier energy term on the free energy density function can be viewed as an increase in the height of the potential barrier between the two minima (refer to the cross-sectional A-B line depicted in Figure 85 (a)).



(a)

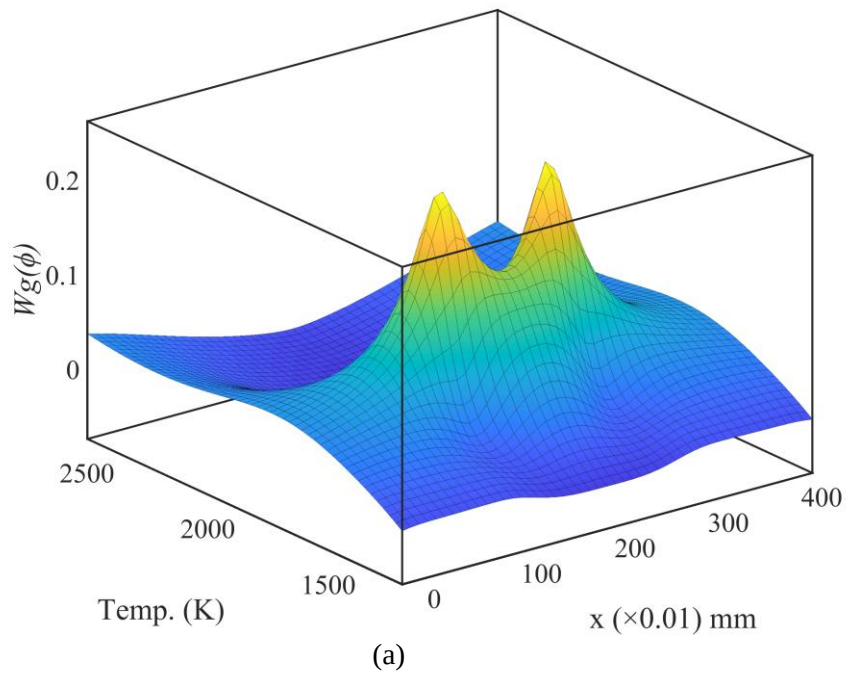


(b)

Figure 86 (a): Effect of the changing parameter l on the phase field graph in the time step 0.25 ms ,
(b): barrier energy term affected by the phase field length scale.

All diagrams are captured across the A-B line shown in Figure 85 (a).

When a material undergoes a complete transition to either a fully liquid or solid state, the thermodynamic driving force of the system approaches zero. However, as the interface between the two phases undergoes changing during solidification, the energy barrier between them increases substantially, adopting the form of a double-well potential function. In Figure 87 (a), the 3D graph of the double well barrier function is plotted against the temperature and the spatial position. Furthermore, the contour represented in Figure 87 (b) shows the spatial changes of temperature in the interval of the phase changing.



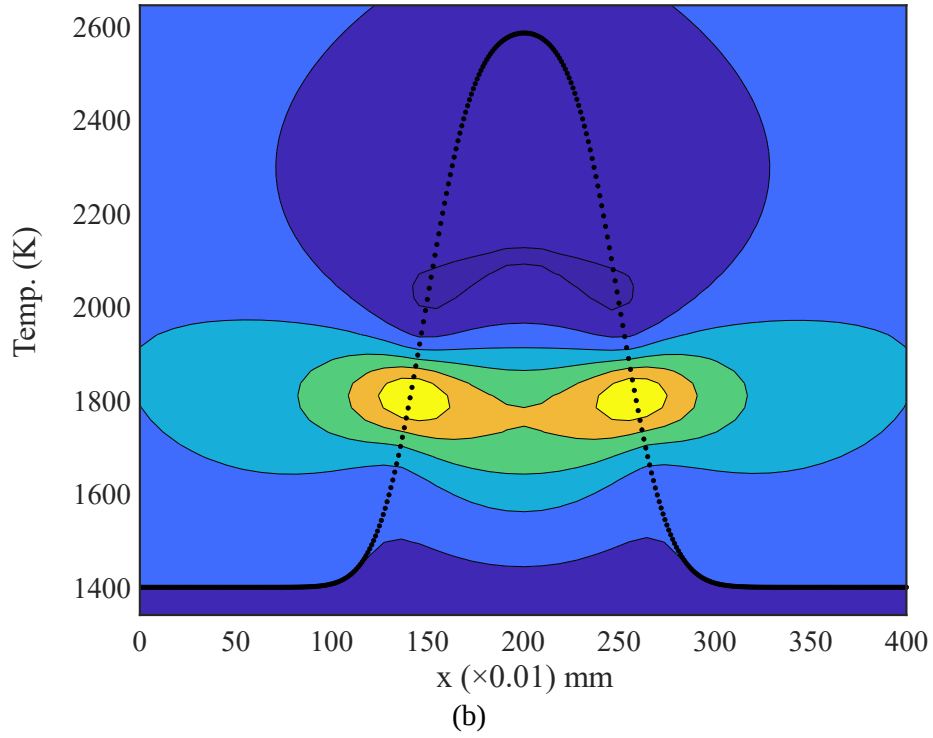


Figure 87 (a) Effect of the phase change on the barrier energy term and (b) spatial temperature changes in the interval of phase changing; the results are obtained at the time step 0.25 ms and using $l = 2$.

All contours are captured across the A-B line shown in Figure 85 (a).

6.2.4.1. Temperature evolution

By adopting distinct values for the phase-field length scale, different responses in terms of the temperature evolution are observed, as shown in graphs of Figure 88 (a). These graphs infer roughly identical temperature distribution for the two selected phase field length scale values and a slight decrease in the peak temperature associated with $l = 2$. This can be further observed qualitatively in the contour plot in Figure 88 (b), where the choice of different length scale parameters resulted in a negligible difference in the solid-liquid interface.

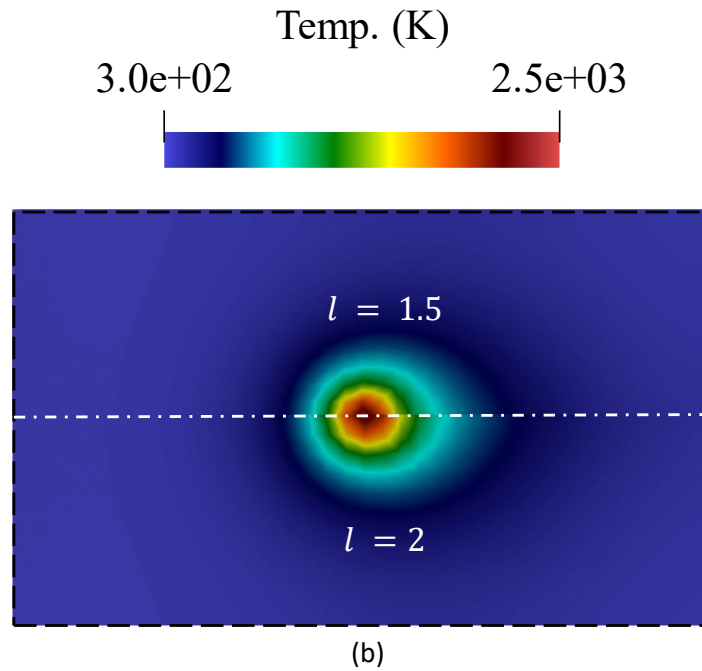
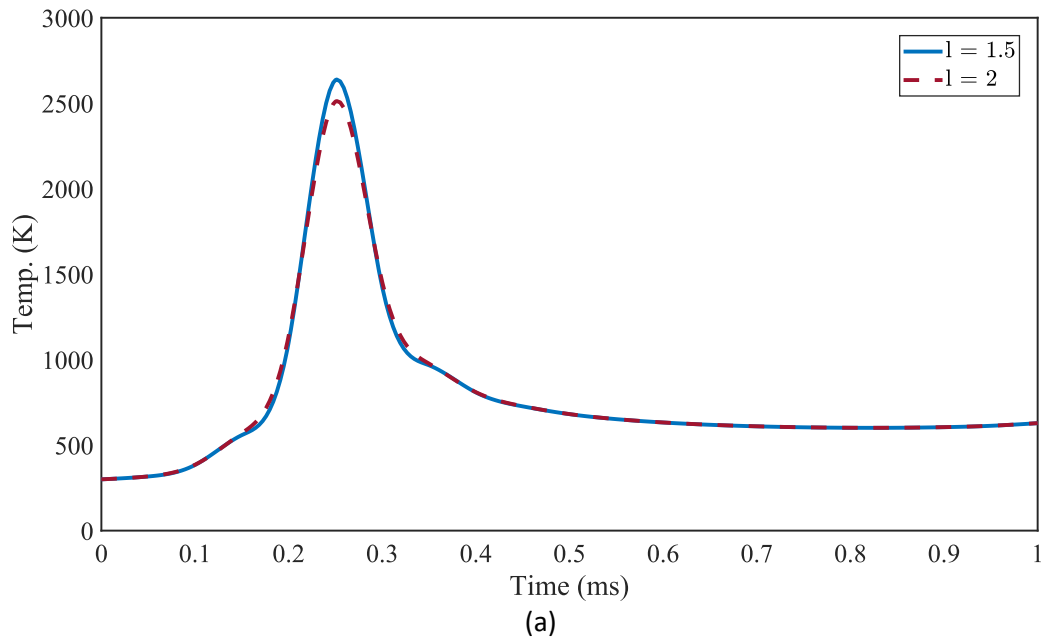


Figure 88 (a): Effect of the changing parameter l on the peak temperature inside the melt pool in the time step 0.25 ms , (b): top view of the temperature distributions for two different values of the phase field length scale parameter.

The maximum temperature graph changes for two values of length scale parameter in the transient solution of the process is shown in Figure 89. Similar to the diagrams observed in Figure 88 (a), slightly smaller maximum temperature was obtained when a larger length scale value was utilized. This data highlights that the maximum temperature within the melt pool exhibits an increasing trend with some intermittent fluctuations. Melt pool instabilities are caused from the increasing temperature as processing

time progresses. These instabilities, resulting from escalating temperature, can have detrimental effects on the quality of the manufactured part, including defects such as porosity, incomplete melting, and inadequate bonding between layers. Therefore, it becomes crucial to effectively control the processing temperature by monitoring or detecting the relevant process parameters associated with the solidification process. It is important to note that the correlation between temperature and melt pool size does not necessarily imply causality and other factors aside from temperature may also be influence the size of the melt pool.

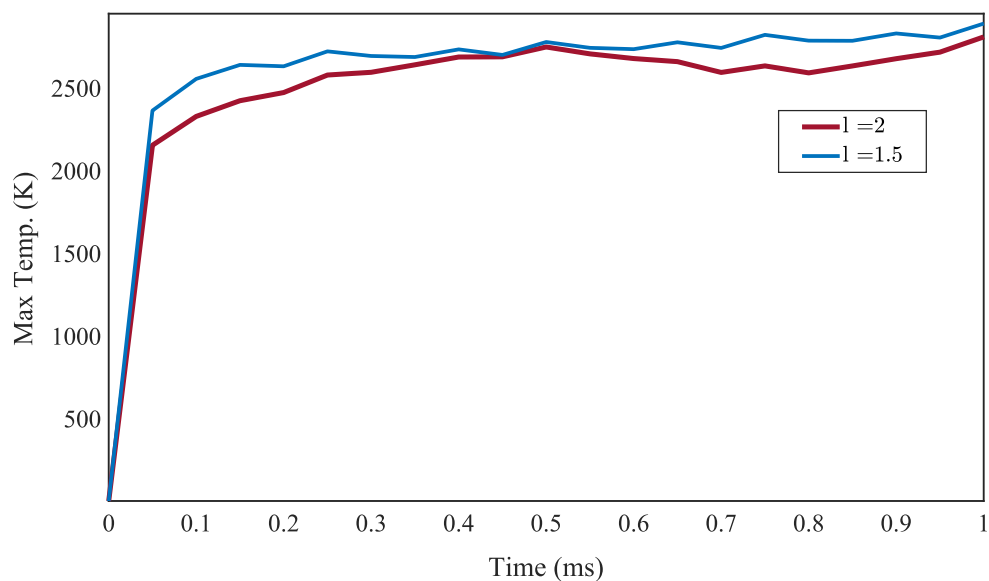
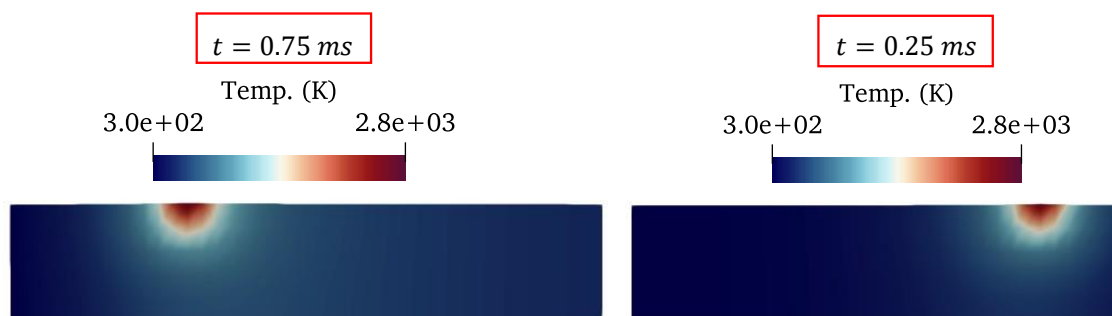


Figure 89 Maximum value of tracked temperature in incremental solution for two phase field length scale parameters.

The contour plots presented in Figure 90 specifically highlight the evolution of the melt pool interface characteristics qualitatively. Figure 90 (a) depicts the temperature contour plots taken at the cross-sectional area of the powder layer and at the time steps $t = 0.25 \text{ ms}$ and $t = 0.75 \text{ ms}$, which are positioned 180 degrees apart from each other. The corresponding plots of phase field parameters at the same time steps are illustrated in Figure 90 (b), which shows the interface of the melt pool located in the powder layer.



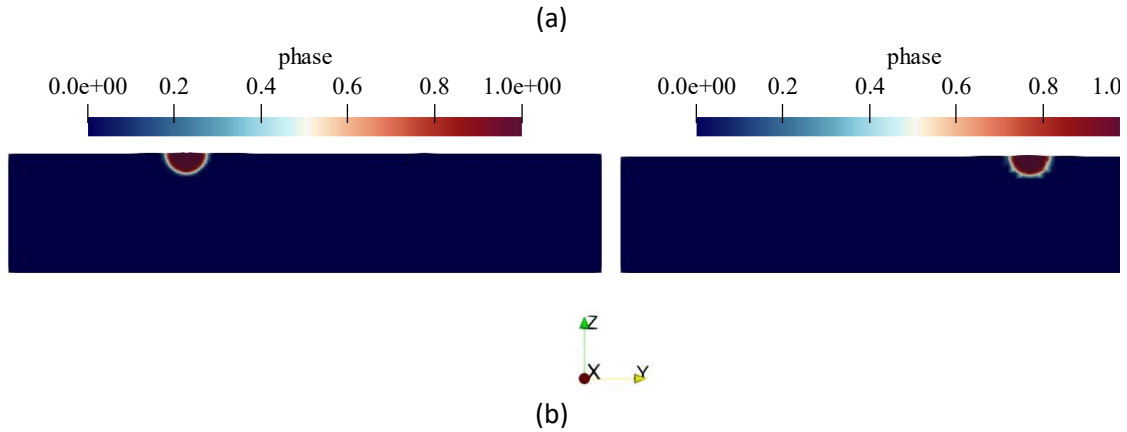
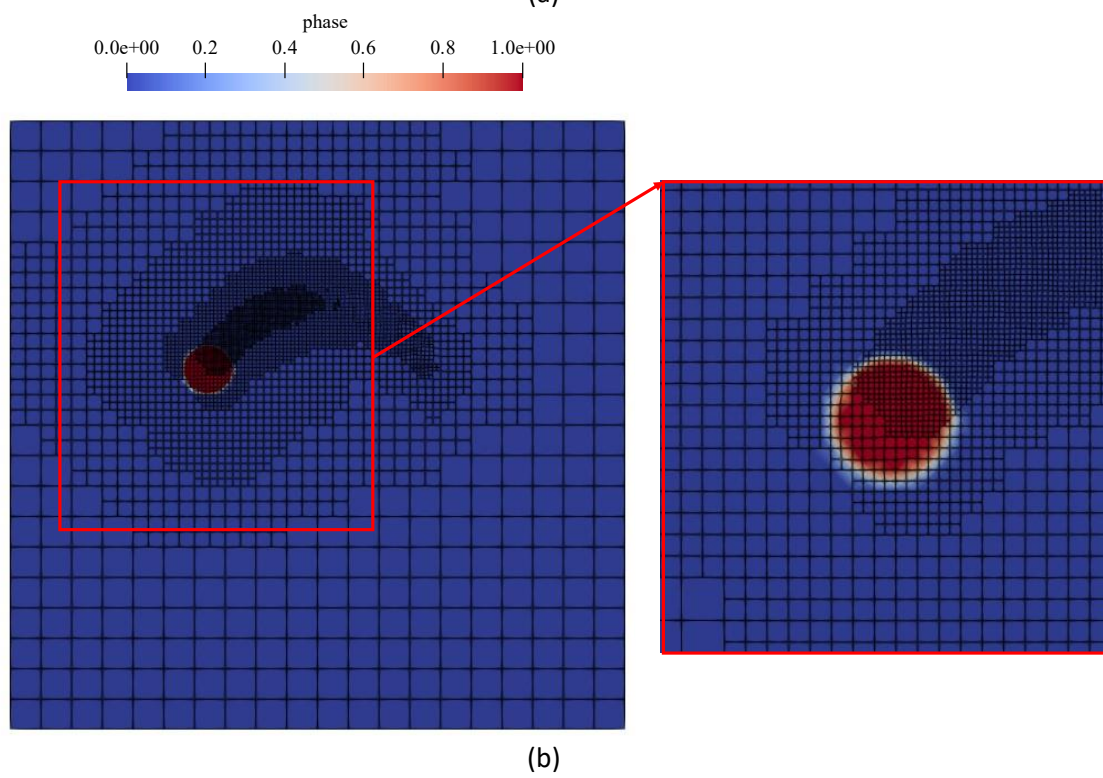
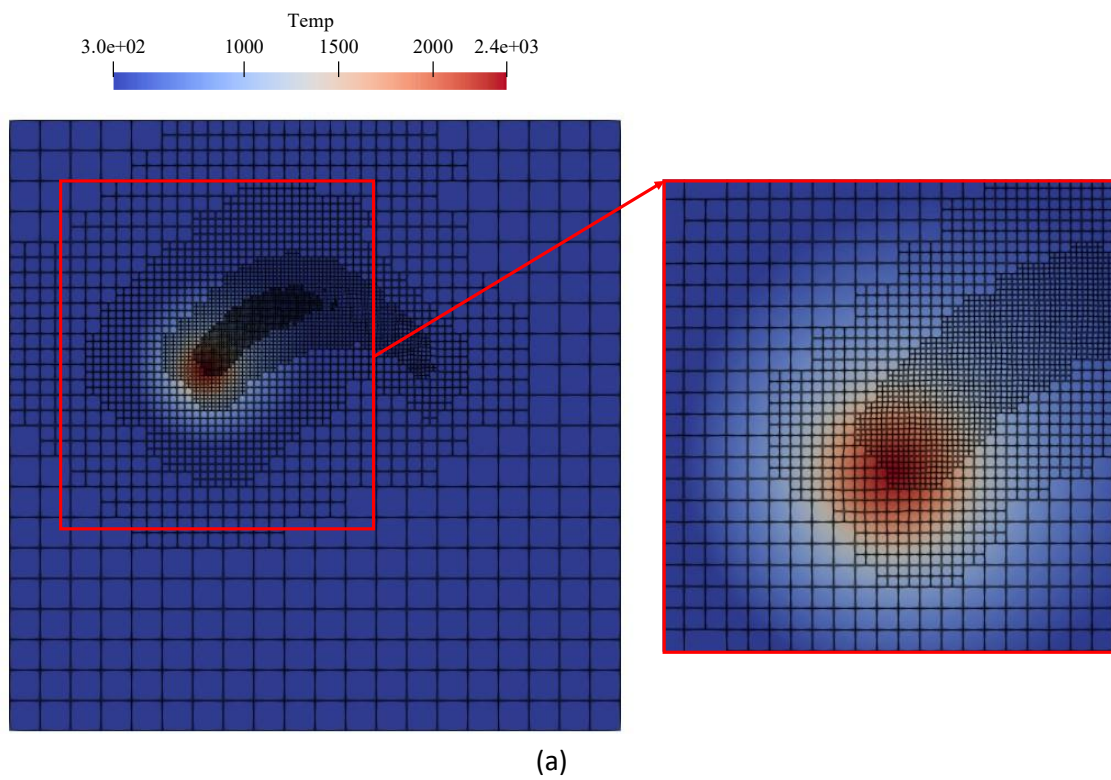


Figure 90 Dynamically decomposed frames for (a): Temperature evolution and (b): phase field evolution in different time steps at the cross-sectional area of the powder layer

6.2.4.2. LibMeh finite element library with adapted mesh refinement (AMR)

The simulation was performed with AMR technique, with refinement based on gradient values in temperature and phase field variable in solidification frontier. This allows for more accurate tracking of the solidification front and dealing with nonlinear phenomena. MOOSE employs adaptivity to automatically refine the mesh in regions of a high estimated solution error for the temperature and phase field variable based on Kelly error estimation [177]. As a laser moves and the temperature front propagates through the domain, the temperature gradients that develop between two adjacent elements increase. As the temperature gradient jump across the element boundaries becomes steeper, the likelihood of error in the solution increases. However, by refining locally the mesh, it is possible to mitigate this error and enhance the solution's accuracy. Thus, the gradient jump error indicator which is capable of estimating the total error at each element, will be used in our modelling. The error-value-threshold scheme then marks elements for local refinement or coarsening based upon a provided maximum/minimum percentage error threshold. Where error values are larger than the maximum acceptable error the mesh is refined and where those error values are lower than the minimum acceptable error the mesh is coarsened. In the area far from the center of the laser heat source, adaptive mesh refinement is needed, while near the maximum laser intensity, the highest refinement level is allocated, allowing for better modelling of the melt pool boundary and more efficient handling of the underlying nonlinear phenomena. The moving laser and the resulted dynamically changing interface, whether powder with molten phase or a phase change in solidification frontier, are tracked by AMR, as shown in Figure 91 (a, b). The melting and solidification interfaces are smeared over two diffused regions, where melting has a larger interface in comparison to solidification. Additionally, the cross-sectional views of temperature distribution and phase separation are shown in Figure 91 (c, d).



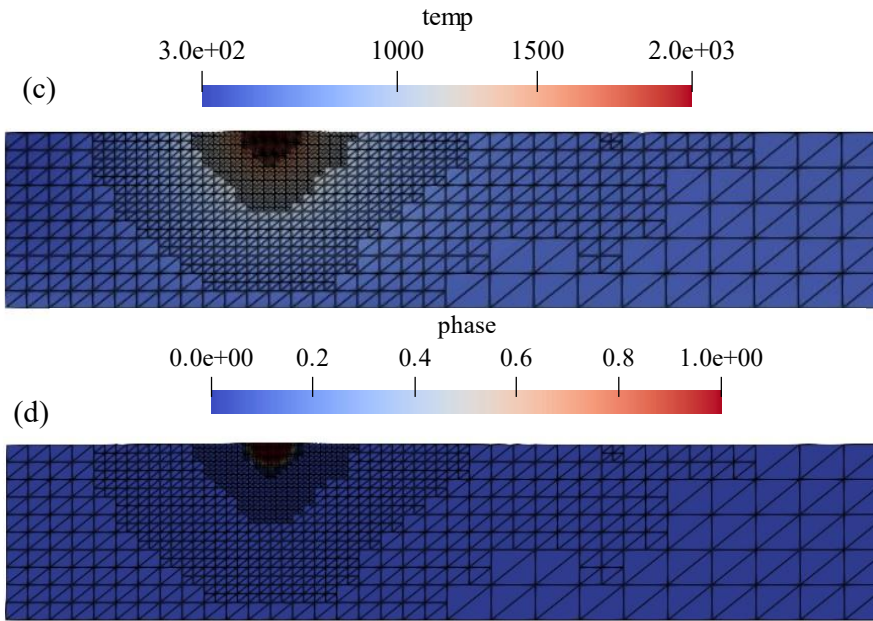


Figure 91 Top view of the element refinement hierarchy with h -adaptivity in domain of melt pool, (a) Temperature distribution and its enlarged view in melt pool, (b) partitioning of the phase changing in melt pool with its enlarged view, (c) cross-sectional view of temperature distribution, (d) cross-sectional view of the phase indicator in the area of melt pool.

Table 14 summarizes the computational cost of these simulations with the AMR technique rather than the fixed refined mesh provided in section 6.2.3.

Table 14 Comparison of computational cost using static mesh scheme and adaptive mesh scheme for a circular scanning track

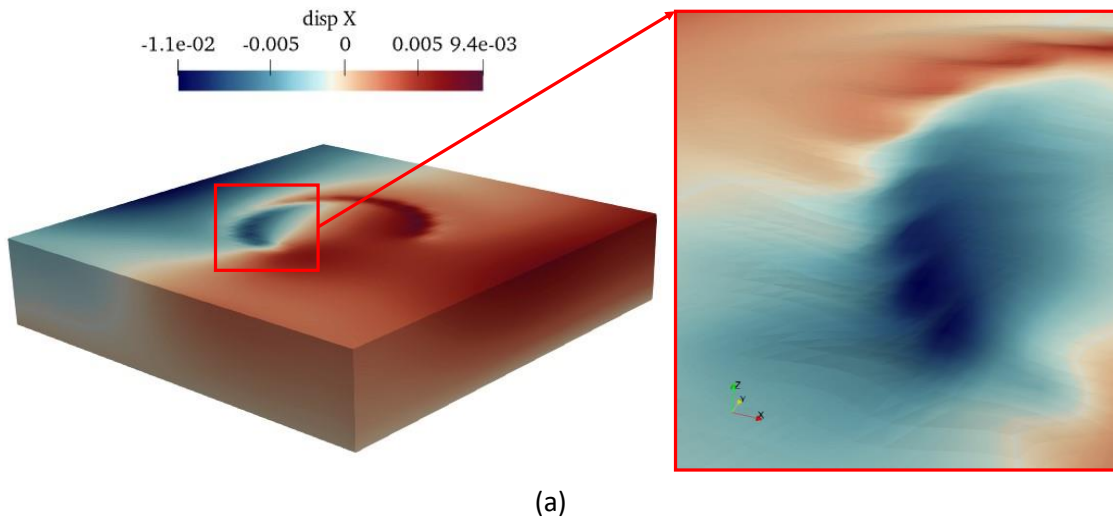
Mesh scheme	Element Number	Node Number	Wall CPU time (s)
Fixed mesh size of 0.0625	512,000	738,290	1417
Adaptive mesh refinement level 7	50,430-136,478	72,871-197,893	513

Table 14 provides insightful information indicating higher computational cost associated with different meshing approaches, revealing that employing fixed mesh size results in higher computational expense compared to an AMR scheme. In the context of a moving laser spot with a prescribed scan speed, it is imperative to adaptively refine the mesh at each time step. However, it is important to strike a balance between the frequency of mesh refinement and the associated computational efforts, which involve tasks such as refining the mesh, renumbering nodes, and interpolating shape functions across different meshes. Moreover, considering the dimensions of the build domain and the desired solution accuracy, employing AMR proves advantageous over the choice of fixed mesh scheme, as this approach optimizes the trade-off between computational efficiency and solution quality. Notably, simulations conducted using the present AMR scheme demonstrate a remarkable reduction in the simulation time, achieving a mere 36%

of the time required by the fixed mesh size scheme, further underscoring the benefits of employing this AMR scheme in additive manufacturing simulations.

6.2.4.3. Thermo Elasto-Plastic Responses

In the PBF fabrication process, the phase and temperature field variables are coupled to equilibrium constitutive formulations. This ensures that at each time step, the updated values of the temperature and phase-field variables, which account for the complex multi-physics involved in rapid heating and cooling, as well as fluctuating steep thermal gradients, are used to compute the displacements and residual stresses in the mechanical problem. This allows for a more accurate and detailed simulation of the PBF fabrication process, providing valuable insights into the impact of temperature and phase changes on the mechanical behavior of the material setting under study. In Figure 92, we present the displacement vector components and a localized zoom at a specific time step, $t = 0.75 \text{ ms}$, during the PBF process, with the plate constrained at the bottom in all degrees of freedom. The contour plots demonstrate the distribution of tension and compression within the material, with red representing the domain under tension and blue indicating compression. These 3D views provide a comprehensive understanding of the of material's volume state at any location within the laser track path as the laser moves in an anti-clockwise direction around the central axis.



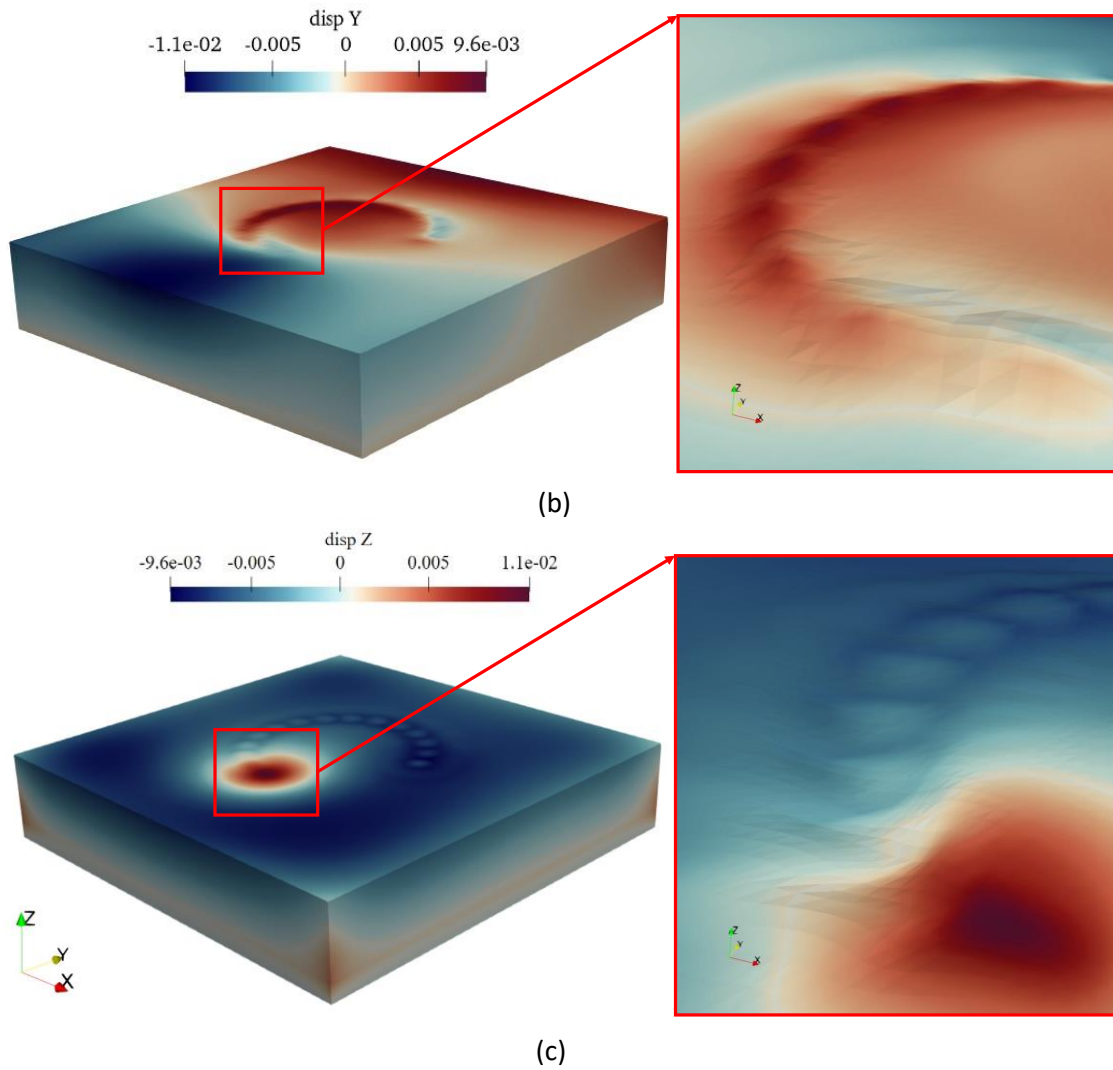


Figure 92 Components of displacement field in (a) x direction, (b) y direction, and (c) z direction; these results are taken using the phase field length scale $l = 2$ and at the time step $t = 0.75 \text{ ms}$.

The displacement values are in mm .

Figure 93 (a–d) presents the 3D map of stress distributions at $t = 0.25 \text{ ms}$ and $t = 0.75 \text{ ms}$, corresponding to the time steps during which melting and solidification occur, respectively. The figures provide a time-progressive view, allowing for a comprehensive understanding of the heating and solidification processes and their influence on the stress patterns. In Figure 93 (a, b) and Figure 93 (c, d), compression stresses are observed in x and y directions, resulting from the transformation of the powder material to molten state. It appears that the laser heat flux exerts a “pushing away” effect on the powder layers during the melting stage. As the powder density undergoes alteration and consolidates, the stresses transition to a tension state. Subsequently, as the printing process progresses, the range of tension stresses in x and y directions increases from 560 MPa to 1200 MPa and from 750 MPa to 1200 MPa , respectively. Meanwhile, the range of compression stress responses decreases from 570 MPa to 540 MPa and from

510 MPa to 480 MPa, respectively, in x and y directions. Along the z axis, which represents the building direction, the stresses at $t = 0.25 \text{ ms}$ or $t = 0.75 \text{ ms}$ are insignificant and reflect the molten phase within the melt pool region.

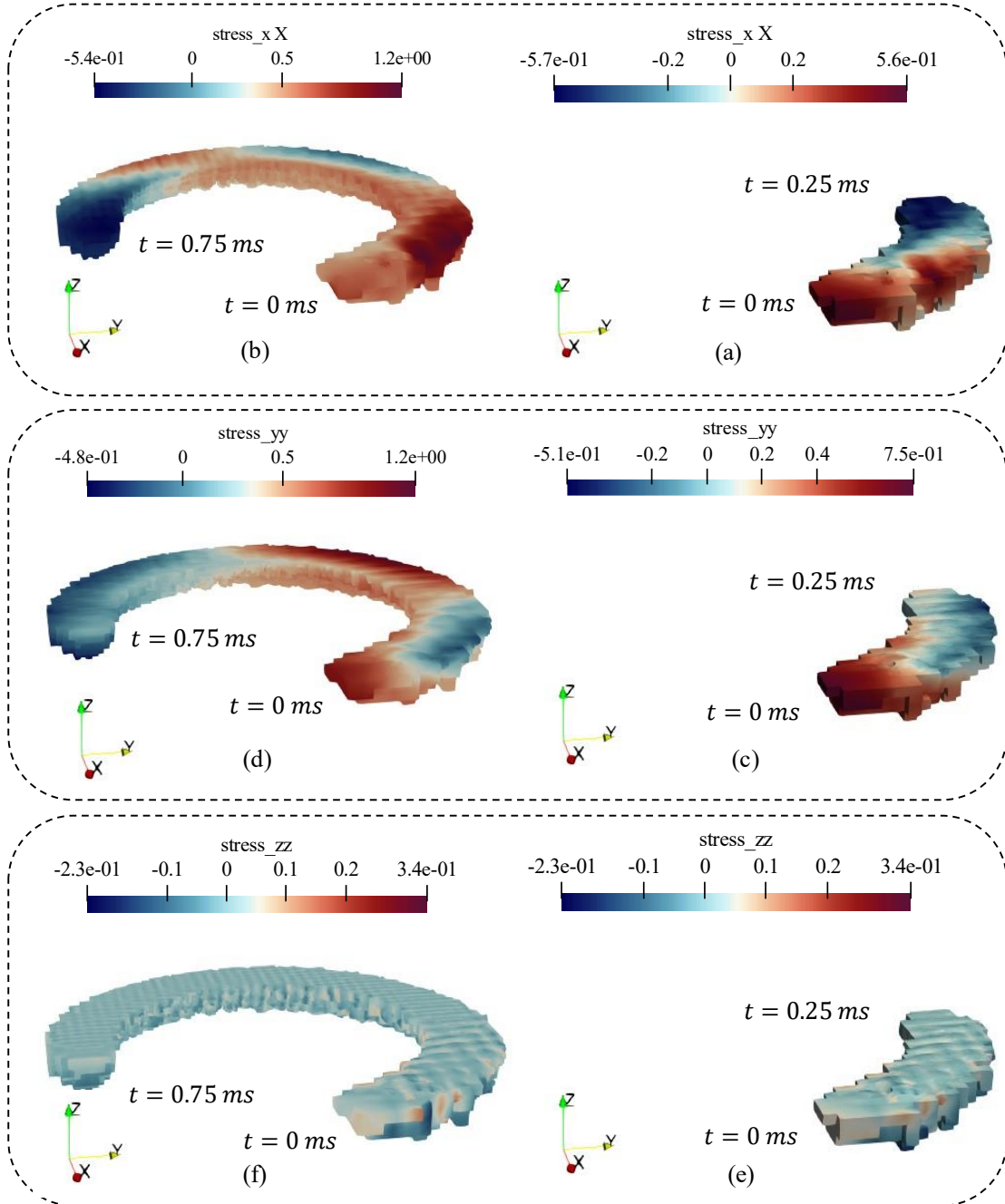


Figure 93 (a-d) Contour plots of stress components in direction x, y and z at $t = 0.25 \text{ ms}$ and $t = 0.75 \text{ ms}$, showing melting and solidification states. (The phase field length scale is set to $l = 2$, and all stress values are in GPa)

Figure 94 (a, b) presents the plot of the von Mises equivalent stress at $t = 0.25 \text{ ms}$ and $t = 0.75 \text{ ms}$, demonstrating an increasing trend in stress distribution throughout the fabrication process. As previously discussed, during the heating phase, the formation of melt takes place, converting the powder material into a liquid phase, with insignificant stresses at the center of the melt pool. Besides, the “tail” region where the substrate interacts with the created molten pool exhibits the lowest stress intensity. Figure 94 (c, d) depicts the distribution of the equivalent plastic strain in 3D view is illustrated during the same time periods. This distribution, not only indicates the occurrence of plastic deformation in the material following the application of heat source, with the maximum values in the plot corresponding to the areas processed by the laser, but it also captures the effect of solidification.

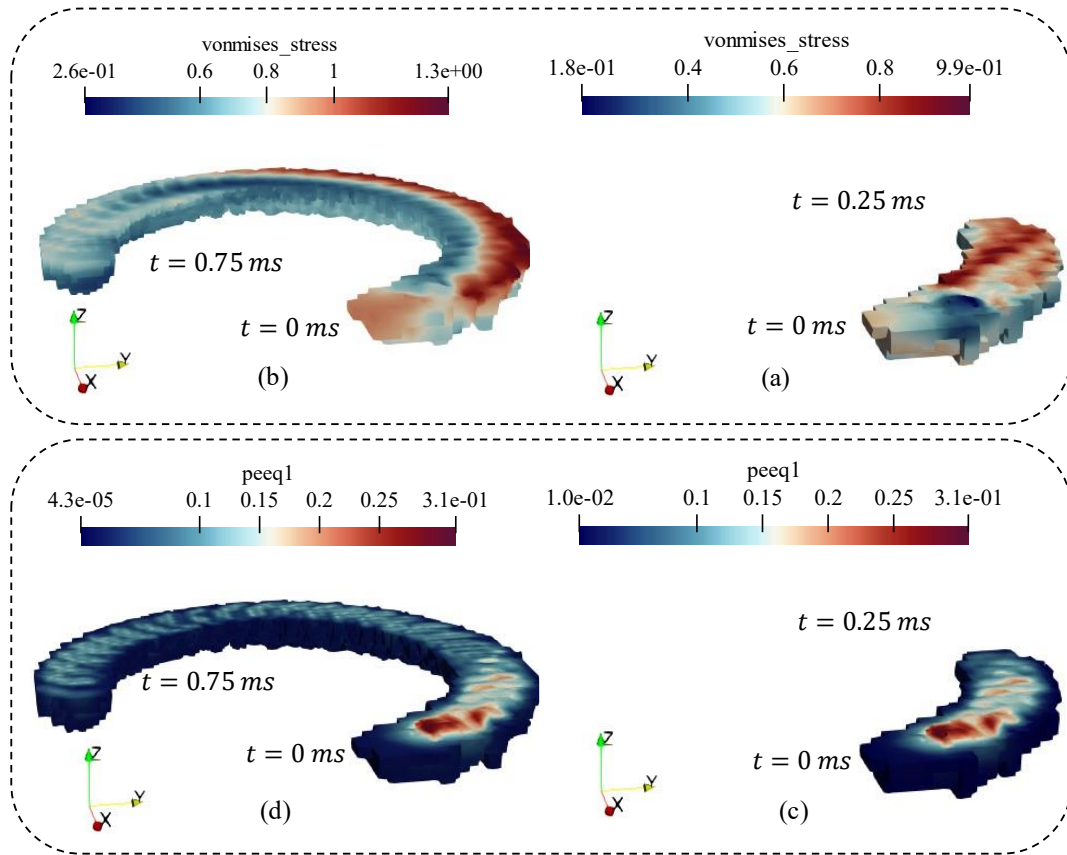


Figure 94 (a, b) Contour plots of von Mises stress and (c, d) equivalent plastic strain frames at the end of the time step $t = 0.75 \text{ ms}$. (The phase field length scale is set to $l = 2$, and all stress values are in GPa).

The distribution of the stress components in terms of the changes in the value of phase-field length parameter at the time step $t = 0.75 \text{ ms}$ is shown in Figure 95. These results are taken at a location below the maximum depth of the melt pool, and it is marked “A” in the figure. These plots reveal the significant influence of the choice of phase-field length scale on the stress distributions at certain time steps of the

heating process. For the case where $l = 1.5$, at $t = 0.25 \text{ ms}$, the stress values in the x and y directions have more fluctuations compared to the case where $l = 2$. Furthermore, significantly higher changes in the stresses in the x and y directions can be observed throughout the heating, while the stress in the z direction remains almost insignificant.

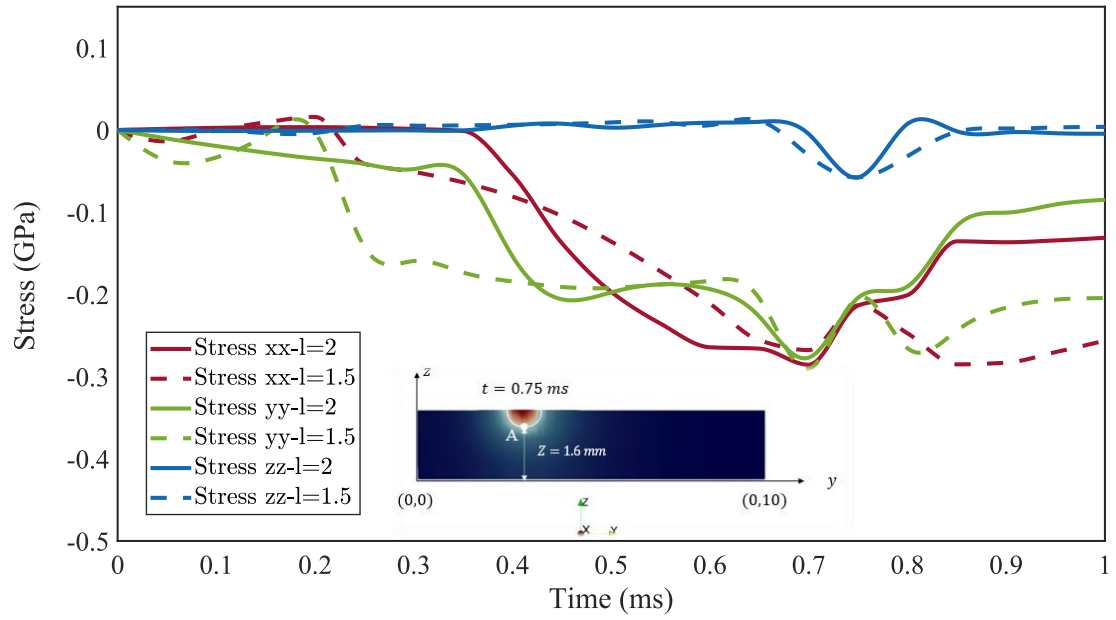


Figure 95 Components of total stresses in the point at the end of melt pool in the time step $t = 0.75 \text{ ms}$ with various phase field length scale.

Chapter 7

Simulation for the control of the process in additive manufacturing

7.1.Introduction

The present chapter aims to design a computational framework to control the melt pool evolution to steer the deposition in DED process using the ABAQUS-implicit commercial environment, which has been described in the previous chapters. To fabricate certified components in AM technology with satisfactory quality, it is vital to implement a control strategy during the deposition process. As a tool, thermal simulations can be used to mitigate the cost of the engineering process by predicting the temperature map throughout the fabrication in the specific deposition area. In this context, the morphology of the melt pool is investigated by segmenting the acquired thermal images from the FEM environment to make it computationally feasible for Reinforcement Learning (RL) adaptation. Highly specialized and accurate discretization schemes have been developed to solve fundamental model equations by FEM. Then, the derived thermal images from the FEM are collected to train a deep RL policy. One of the central motivations for the combination of precise FEM modeling with RL is that they are powerful for learning from experience but, at the same time, strongly profit from domain knowledge in the form of physical models. Besides, even though AI techniques are novel, it is sometimes difficult to apply them, and, admittedly, often non-trivial to properly integrate our understanding of physical processes into the learning algorithms. Thus, here, the RL method framework uses image segmentation in 2D thermal maps for feature extractions, like melt pool morphology and a peak temperature of the melt pool area on the top surface of the substrate. In this scenario where a solver repeatedly targets cases from a certain well-defined problem domain, it can make a lot of sense to train a neural network with repeated solvers. Considering that the usage of RL for technological process control is still in its early stages of development, this research has tried to overcome the obstacles with the training process which may be time-consuming and data-intensive in real-world; building up a robust controller to improve the stability of the melt pool, and enhancement of the generalization capabilities of RL controllers by using approaches in transfer learning from simulation to the real-world application. Figure 96 illustrates the scheme of the proposed research framework.

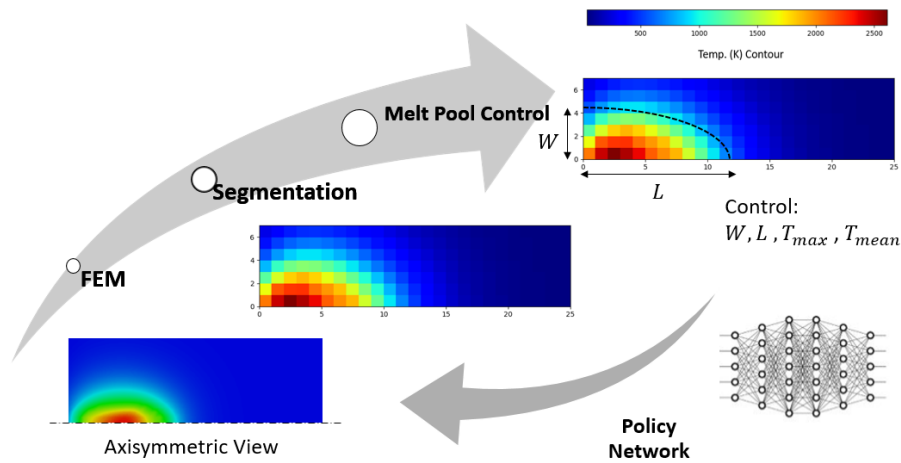


Figure 96 Representative temperature contour and molten pool geometry transition from physics-driven FEM environment to RL agent as a closed-loop environment.

7.2. Effect of the process parameters in DED

Due to the fact that laser-based manufacturing procedures require a variety of processing parameters and complex temperature cycles, even a minor change in the processing environment can affect the clad quality, imperfections, and accuracy of the printed parts [178,179]. The induced defects may significantly impact the fabricated part performance. The study of deposition physics can reveal the complexity of the process. As reported in [180] nineteen parameters (laser beam power, scan speed, beam spot diameter, powder layer thickness, powder mass flow rate, carrier and shielding gas pressure, powder particle size and shape, standoff distance, thermal conductivity of powder and substrate, hatch spacing, percentage of overlapping, and interlayer ideal time) are listed by the authors as the process parameters that could impact the manufacturing process. To achieve the desired qualities, it is essential to build quantitative relationships between the process parameters and the interested properties of the final parts such as porosity, residual stress, microstructure, etc. Moreover, some environment-dependent parameters depend on the aforementioned process parameters, making the entire process even more complex. Besides, clad morphology, surface roughness, dilution value, microstructural properties, mechanical behavior, and metallurgical features are greatly influenced by small changes in those parameters. To illustrate it, in Figure 97 different input parameters and physical phenomena involved in D are compiled. As a result, it seems intricate to investigate the DED process with all the process parameters, and in the following section, modeling is just conducted with a short number of key parameters.

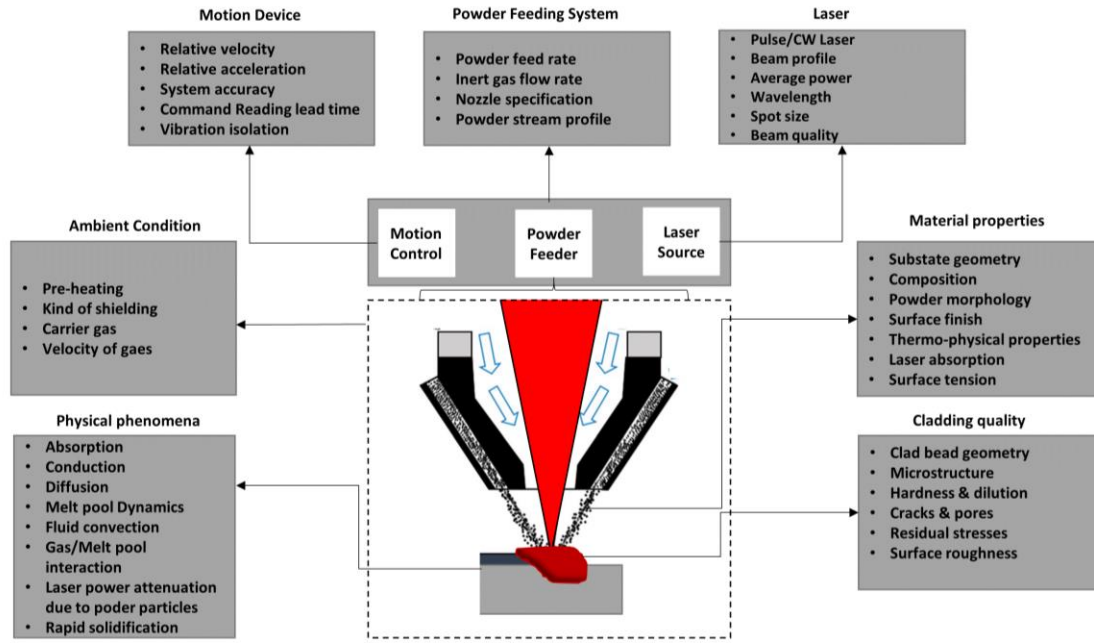


Figure 97 Clad quality, different input parameters, and physical phenomena involved in deposition with powder blown method of laser cladding [179].

7.3.Reinforcement Learning (RL)

During the last decade, RL has emerged as a method of addressing complex control environments in relatively high-dimensional dynamic spaces [181,182]. RL is a self-learning method that is capable of iteratively improving on an initially random control policy by gaining experience by observation an environment, whether real or simulated. Deep reinforcement learning can dynamically adapt to previously hidden process parameters, enabling it to harness a richer set of data to inform the decision-making agent. Taking advantage of the promising ability to provide data for high dimensional state spaces, it reveals capability in the optimization of complex cases and preparing a sophisticated control policy to address a key mechanism of the effect of process parameters in outputs. The environment and the agent are the two main components of the RL setup. The environment receives actions, a , from the agent while providing it with observations in the form of states, s , and rewards, r . The observations represent the fraction of the information from the environment that the agent can perceive. A stated reward function, usually suited to the environment, determines the incentives, which may include a score, a penalty for erroneous behaviors, or a bounty for successfully completed tasks. The objective of reinforcement learning, in a simple way, is to maximize the long-term reward according to Equation (7.1).

$$\arg \max_{\theta} \mathbb{E}_{a \sim \pi(\cdot; s, \theta_p)} \left[\sum_t r_t \right] \quad (7.1)$$

where the reward r_t at time t is the result of an action a performed by an agent that achieve a state s . The agents choose their actions based on a neural network policy, which decides via a set of given observations. The policy $\pi(a; s, \theta)$ returns the probability for the action, and is conditioned on the state, s , of the environment and the weights θ [183]. The basic goal of RL during the learning process is to raise the cumulative reward along with each episode by combining information from the state, action, and matching rewards. Multiple algorithms have been developed to achieve this goal in several environments, which can be roughly split into two classes: value-based techniques and policy gradients. Q -Learning and other value-based approaches work by optimizing a state-action value function. With the advantages of deep learning, Deep- Q -learning algorithms are considered one of the core concepts of RL. In this scenario, with a given state s and action a , a function or neural network (NN) is used to predict the average cumulative reward for the rest of the episode, i.e., $Q(s, a)$. Following that, actions are chosen to maximize Q given the current situation. On the other hand, actor-critic methods, combine components from both approaches. The actions created by a policy network are graded using the changes in state potential. These values are given by another neural network and approximate the expected cumulative reward from the given state. One example of this family of methods is Proximal Policy Optimization (PPO) [184]. As an actor-critic approach, it is necessary to train two interdependent networks. The actor's goal is inextricably linked to the output of the critic network - which indicates which acts are worthwhile, and the critic is inextricably linked to the actions generated by the actor network - this determines which states to explore. The actor computes a policy function returning the probability distribution for the actions conditioned by the current network parameters θ and a state s . As mentioned before, the training procedure computes a certain number of weight updates using policy evaluations with a fixed previous network state $\pi(a; s, \theta_p)$ and in intervals re-initializes the previous weights θ_p from θ . ϵ defines the bound for the deviation from the previous policy. In combination, the objective for the actor is given by the Equation (7.2).

$$\begin{aligned} & \arg \max_{\theta} E_{a \sim \pi(\cdot; s, \theta_p)} \\ & \left[\min \left(\frac{\pi(a; s, \theta)}{\pi(a; s, \theta_p)} A(s, a; \phi), \text{clip} \left(\frac{\pi(a; s, \theta)}{\pi(a; s, \theta_p)}, 1 - \epsilon, 1 + \epsilon \right) A(s, a; \phi) \right) \right] \end{aligned} \quad (7.2)$$

PPO was designed to restrain instabilities promoted by the network's interdependence. The goal is to limit the impact of individual state value estimates on the change in the actor's behavior during learning. These value estimates form the loss of the policy network, given by the change in reward potential by the chosen action. When working on continuous action spaces, PPO is a

frequent choice because it produces strong results with a consistent learning progression while remaining simple to apply [185].

7.4. Algorithm implementation

In order to train a RL agent to control the melt pool morphology and temperature, ABAQUS simulation input and output needs to be linked to an RL environment. In line with that, a custom OpenAI Gym environment was developed, and with stable-baselines3 [186] was used to train a PPO model. Therefore, a standard customized environment has been developed to facilitate the easy and reliable implementation of already proven "free RL algorithms" using stable-baselines algorithms in various other applications. Using this framework, it is possible to vectorize environments for a faster learning process, normalize the reward and observable state, and apply standard RL algorithms. Figure 98 illustrates how OpenAI Gym and Stable-baselines can be applied to the described control with ABAQUS.

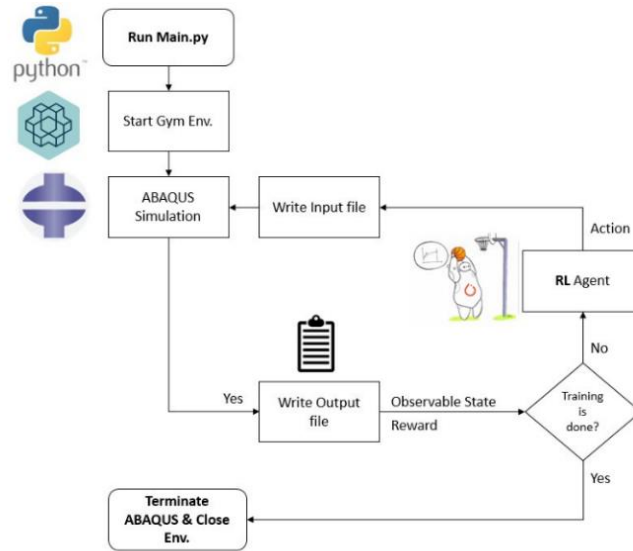


Figure 98 Outline of the workflow during training. to stand out, the interaction between ABAQUS and OpenAI gym uses functions developed to write and read information from both frameworks.

The implementation of the mentioned approach requires the definition of the observable state and reward, as well as the communication of the action with the environment of ABAQUS, as shown in Figure 99 (a). Hereby, the observable state-space is assigned to the calculated nodal temperature on the 2D map perpendicular to the laser axis. That is, the observable state space is represented by 2D heat maps of temperature distribution surrounding the local position of the laser window as shown in Figure 99 (b). The reward is calculated based on the observable state where the area and melt pool length is evaluated, as well as the mean temperature.

This data is obtained when implementing the mentioned approach, which requires defining the observable state and reward, as well as communicating the action with the ABAQUS environment, as shown in Figure 99 (a). Hereby, an observable state-space is assigned to the calculated nodal temperatures on the 2D map perpendicular to the laser axis. That is, the observable state space is represented by 2D heat maps of temperature distribution surrounding the local position of the laser window as shown in Figure 99 (b). The reward is calculated based on the observable state where the area and melt pool length is evaluated, as well as the mean temperature. This data is obtained at each step using OpenCV [159], where a threshold temperature of 2000 °C was defined for melt pool segmentation.

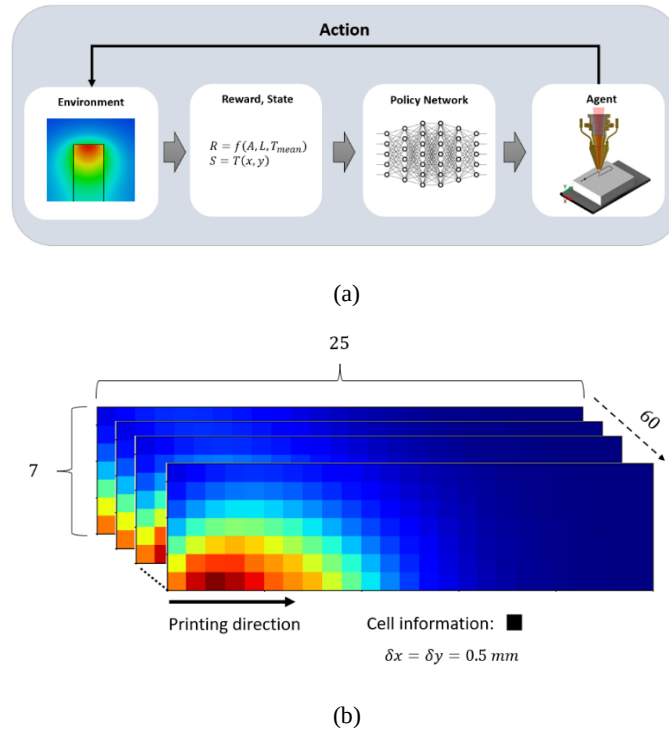


Figure 99 schematic of RL framework, (a) an agent selects an action, based on the current state s and the policy π mapping each state to an action. the action is deployed in the environment, influencing the environment, modifying its state, and producing a reward based on this influence. the policy is updated based on reward, with the end goal of maximizing the cumulative reward. (b) provided environment by ABAQUS.

The reward function quantifies the performance in previous actions with the actual observation. In line with the control of melt pool morphology and temperature, the first reward term is defined as the sum of absolute errors between target length and width and current values based on equation (7.3), where a relatively small and balanced reward is sought for the three variables:

$$r_{i+1_1} = -\left(\lambda_1|\epsilon_{area}|_i + \lambda_2|\epsilon_{width}|_i + \lambda_3|\epsilon_{T_{mean}}|_i\right) \quad (7.3)$$

in which $|\epsilon_{area}|_i$, $|\epsilon_{width}|_i$ and, $|\epsilon_{T_{mean}}|_i$ represent the absolute value of the error functions, between the current value of the mentioned parameters with the target utopia in every iteration. The multipliers $\lambda_{1,2,3}$ indicate the weighting factors of each singular error function. To test the training a simpler reward function, named r_{i2} in Equation (7.4), was defined, where only the maximum temperature is evaluated.

$$r_{i+12} = 1 - \lambda_4 |\epsilon_{T_{max}}|_i \quad (7.4)$$

In this equation $|\epsilon_{T_{max}}|$ is the absolute value of error between the maximum measured temperature and the set point value, in this case defined as 2600°C , and λ_4 is a weighting factor of the error. Despite being a simple reward function, it allows obtaining a positive value for each observation, making the agent look for a solution that is not divergent. Moreover, the temperature is confined to the boundary range to avoid exceeding the vaporization temperature. The action space is defined as the laser power to alter in range of $[-1, 1]$ Equation (7.5) illustrates the function of laser power (W) and feeding back action from consecutive time-increments.

$$P_{i+1} = (2 + a_i) * 10^3 \quad (7.5)$$

where P_{i+1} is the power based on the prescribed action for the next iteration regarding, and a_i represents the action of the previous incremental solving. The range of action chosen is the recommended by SB3 as a gym space box. With this action execution, the laser power range will vary in the range of $[1000\text{ W}, 3000\text{ W}]$. Algorithms 1-3 (Figure 100) show the implementation of RL in a FEM framework for solving the transient heat equation in a custom Gym environment. Algorithm 1 demonstrates how the customized environment was developed to interact with the write/read files from ABAQUS; Algorithm 2 presents in a simplified way the use of Stable Baselines3 for model training; and Algorithm 3 shows the connection of ABAQUS with the RL environment and the functions of the physical model created for the DED process resorting to FORTRAN subroutines.

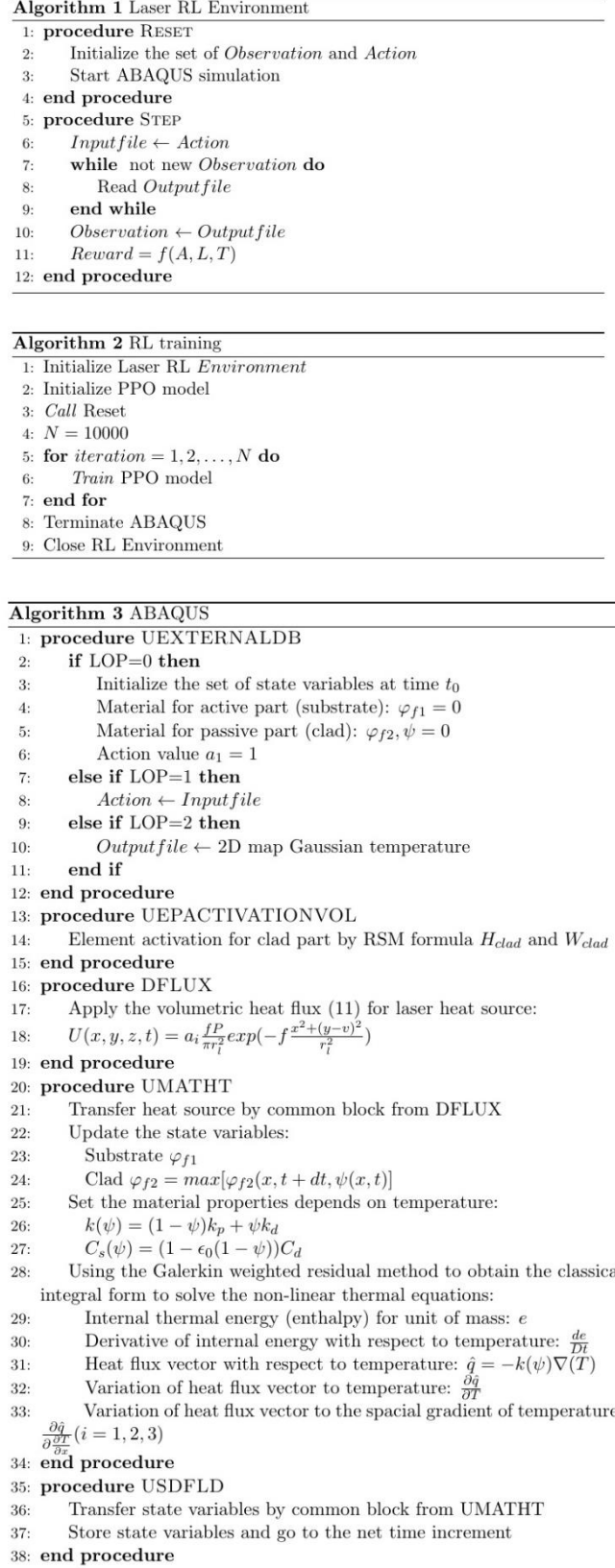


Figure 100 Applied algorithms for RL training.

The OpenAI Gym environment allows a straightforward interconnection with ABAQUS since it solves temporal increments of the process simulation (steps) and a sequence of steps making a

continuum scenario. In the current study, the use of files for communication between the two systems is possible as the simulation takes 1~2 (s) to solve each time increment with a CLUSTER equipped with 32-core CPU provided by FEUP across all nodes. As the time for each increment is considered too high, a new computational and communication architecture is required. Therefore, this capability enables the system to perform hundreds of thousands of iterations in a timely manner, allowing the RL agent to learn traditional and potentially innovative printing strategies while considering the dynamics of the process.

7.5.Results and Discussions

In this research, RL framework is used to create the sophisticated control policy that addresses a critical mechanism of melt pool observation to prevent the defect formation induced by melt pool instabilities. The variation of the melt pool morphology area on the 2D map is searched during the melting process in DED on the substrate. To train the agent of RL, a numerical technique for the thermal part of DED process simulation, using ABAQUS-implicit, was proposed based on the phase-field concept to create a 2D thermal map of transient phenomena. It is worth to be noted that the simulation results with the proposed strategy were validated in the previous research [24]. The analyses of the calculation results are summarized in the following sections.

7.5.1. Observation Space

In additive manufacturing process simulation, adapting adequate spatial and time discretization to achieve accurate results in trading off the computation cost is a vital factor. In this study, the dedicated mesh grid size is 0.5 (mm) and the time step is 0.05 (s) so as to verify the Courant-Friedrichs-Lewy (CFL) stability condition while achieving an affordable computation cost. The segmentation is performed using openCV-python functions to mimic the finite element simulation discretization to obtain data such as melt pool area, length, and width, mean and maximum temperature for further definition of the reward function. Due to the dependency of the grabbed threshold border size on the mesh size, Figure 101 (a-d) was utilized to evaluate the effect of the threshold temperature on the size of the melt pool. In Figure 101 (a, b), the size of the segmented melt pool at the start and end of the simulation is shown at the head and tail of the substrate, respectively, with a threshold temperature of 1770 °C. Furthermore, Figure 101 (c, d) illustrates the same area with a different threshold temperature set at 2000 °C. The reported values are presented in detail, and a comparison with the experimental study from section 5.2.3 reveals that a threshold temperature of 2000 °C is more compatible with the real-world value. As a result, it has been chosen as the appropriate threshold temperature for the remainder of this study.

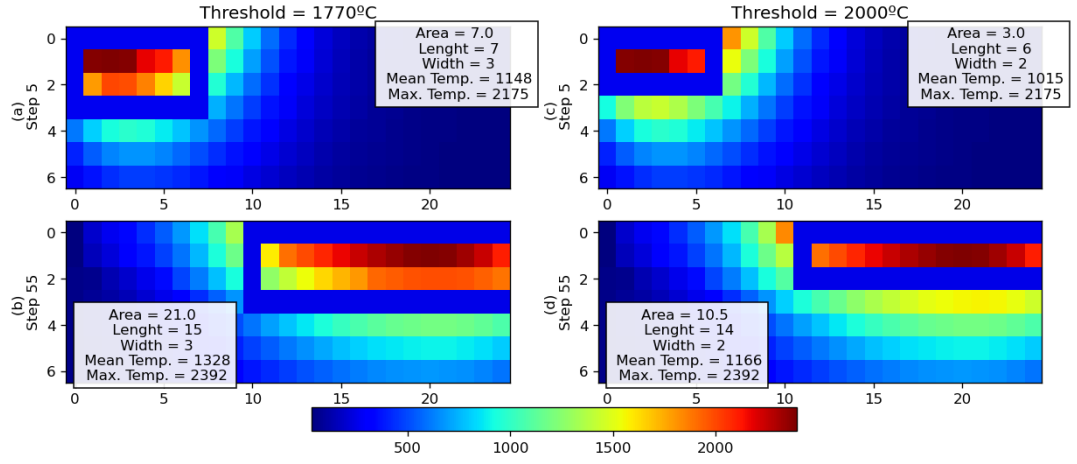


Figure 101 Contrivance in selecting the border temperature to compensate the rough pixel effect, (a) in step number 5 with a threshold temperature 1770 °C at the head of the substrate, (b) in step number 5 with a threshold temperature 1770 °C at the tail of the substrate, (c) in step number 55 with a threshold temperature 2000 °C at the head of the substrate, (d) in step number 55 with a threshold temperature 2000 °C at the tail of the substrate.

7.5.2. RL model training

As mentioned in section 7.4, two different approaches were applied to the reward function including one with a negative reward and several variables in Equation 7.3; and another where the rewards are positive, assessing only the maximum temperature based on Equation 7.4. In this study, the PPO models were trained with 10k iterations and a learning rate of $1.0e^{-4}$ for:

- (A1) with negative rewards and where $\lambda_1 = \lambda_2 = 1$ and $\lambda_3 = 0.1$
- (A2) with positive rewards and $\lambda_4 = 1$
- (A3) with positive rewards and $\lambda_4 = 6$

The plot in Figure 102 illustrates the mean rewards curve during training for agent A1. Initially, the agent starts in a random state, but from 4000 steps onwards, there is a noticeable upward trend in rewards. It is important to mention that this agent has episodes of fixed length. This decision was made to address instances where the agent learned to deviate from the simulation solution by alternating between the maximum and minimum actions for a few steps.

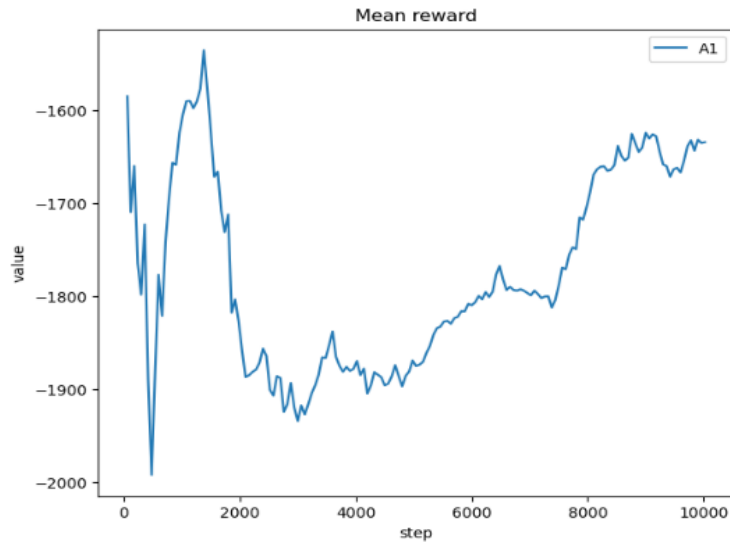


Figure 102 Mean reward curve for agent a1 during training with negative rewards.
Vertical axis is temp in kelvin unit.

Figure 103 (a, b) illustrates the curve of average reward and mean length of an episode with training agents A2 and A3. As for the training of agent A1, after 4000 steps the curves show a growing trend.

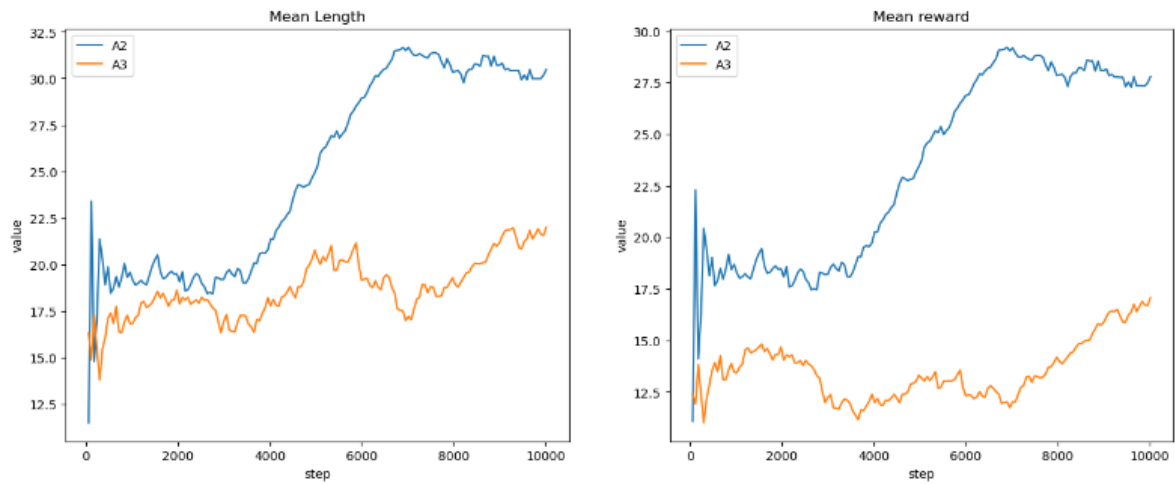


Figure 103 (a) mean episode length and (b) mean reward curve for agents a2 and a3 during training with positive rewards.

Vertical unit is mm^2 .

The usage of a positive reward not only teaches to control the temperature or morphology of the melting pool but also encourages to have a longer episode length, consequently translating into a shorter training time. Furthermore, even though in all of them the reward was normalized, it is recommended to use a small reward value. In conclusion, agent A2 presents in general a better

curve during training, because despite only reaching an episode length value of 32 out of 60, it manages to maximize the reward value closer to the maximum possible one.

7.5.3. RL-based melt pool control

By applying the PPO RL algorithm described in section 7.3, the area of the melt pool formed during a single layer cladding of the manufacturing process with DED is dynamically optimized. In this research, the velocity of the laser resource and the feeding rate of the powder stream are fixed to 10 mm/s and 15 gr/min , respectively in the finite element simulations. As the RL algorithm can discover a policy that changes the process parameter over time, the performance of the laser power is controlled by a policy based on the observation space, the melt pool morphology and the temperature, during the entire melting process.

Figure 104 (a) displays the melt pool dimensions and its isothermal temperature boundary without applying the feeding form RL controlling policy. Figure 104 (b) illustrates the molten phase surrounded by a mushy melt/dense domain and fully dense domain for the same case.

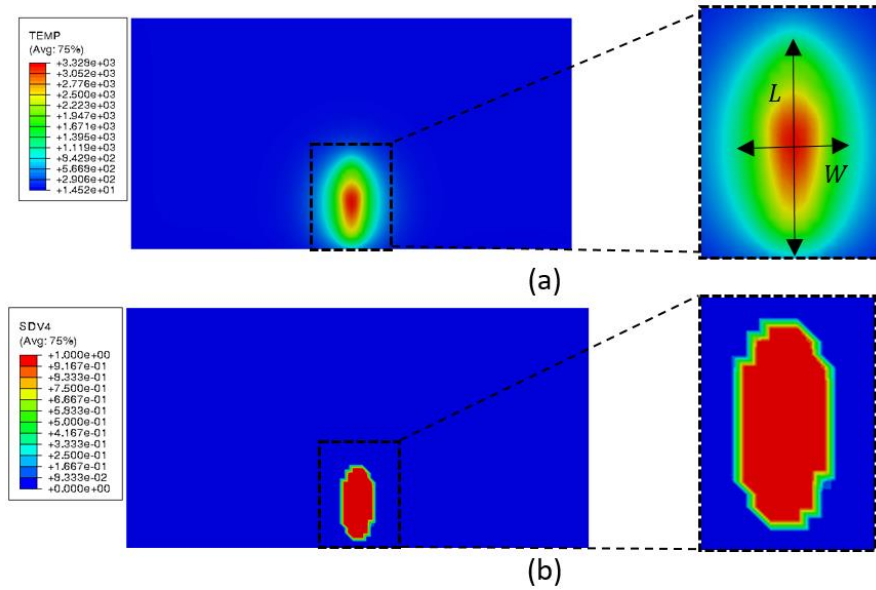


Figure 104 Morphology of melt pool domain without controller for laser velocity 10 mm/s and feed rate 15 gr/min , (a) temperature distribution with its enlarged view, (b) phase-field variable to detect the domain of liquidus/solidus border with its enlarged view.

The vectorized 2D thermal maps are segmented and the threshold boundary of the melt pool is detected as the area of interest to investigate the maximum temperature and dimensions of the melt pool, including length and width. The dynamic thermal frames derived from FEM are evaluated for the respective time-step increments during deposition. Due to the long-time exposure to the laser heat source, the temperature in the structure is accumulated and not only

leads to an increase in the peak temperature but also a significant increase in the melt pool area resulting from the proportional growth of length and width of the melt pool.

Figures 105 (a-f) show the graphs of the aforementioned variables calculated by openCV with/without control. The lack of control, here, literally means printing with the constant dedicated value for laser power, 2000 W. Figure 105 (a) illustrates the action taken by the agents in a full evaluation episode. By increasing the temperature in the melt pool, which is shown in Figure 105 (e-f), it is expected that the agent starts with a positive action and then decreasing the laser power until some value. This behavior was achieved with action A2 but also A1 is slowly decreasing the action value. Figure 105 (b, c) show the size fluctuation of the melt pool for area and width, respectively, through time, which is evaluated by continuum frames of the melt pool. Obviously, it can be seen after the implementation of policy on the ABAQUS-implicit, that the area has less fluctuation and a tendency to approach the smooth behavior. Figure 105 (c) displays the recorded melt pool width, indicating the need for a finer mesh size in the melt pool region to achieve more accurate results. An alternative approach could involve implementing an adaptive mesh algorithm specifically in the melt pool area, although this was not explored in this study due to computational constraints. Additionally, Figures 105 (e, f) demonstrate the increasing trend of the peak temperature and its mean value, providing further evidence of temperature accumulation phenomena. It is important to note that for agent A1, the policy focuses on tracking the mean temperature value, with the maximum temperature being an indirect consequence of this approach. While agents A2 and A3 were trained using a reward function that evaluates the maximum temperature, additional training is necessary as A2 displays some promising control behavior only up to step 30. To shed some light on the effect of using RL on the simulation environment, the results of the simulation are prepared in the same graphs, where the mean temperature is under control to avoid exceeding the specific value and its significant effect on the peak temperature inside the melt pool border.

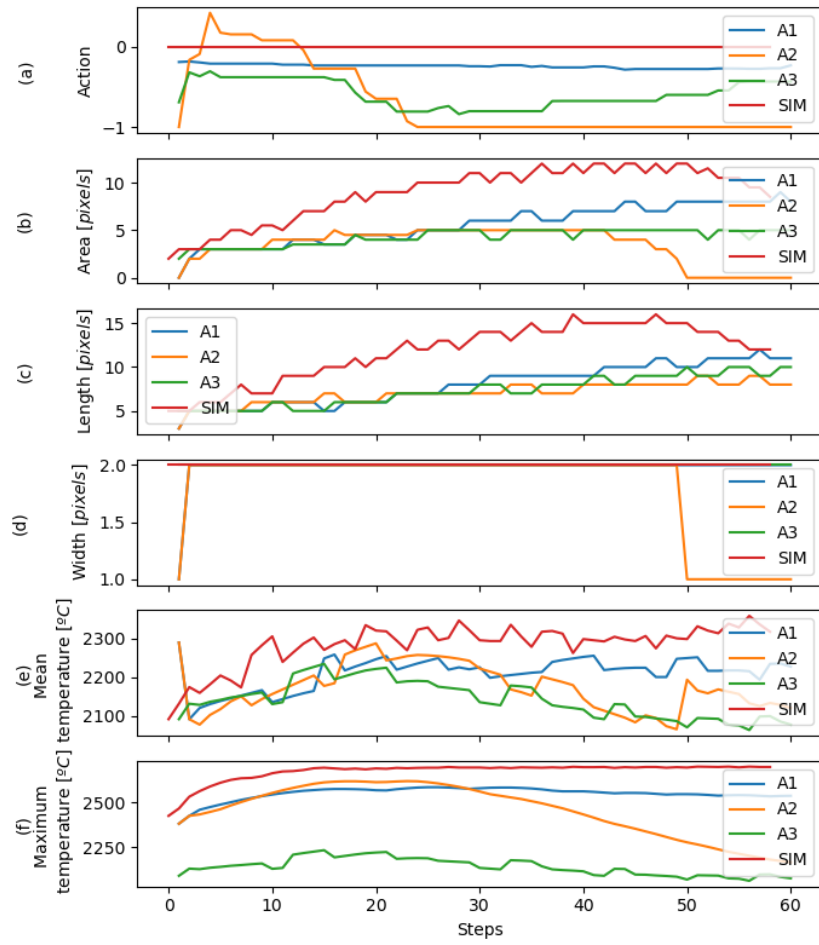


Figure 105 Melt Pool identifications achieved following the rl policy: (a) action of the agent, (b) area of melt pool on the top view, (c) width of melt pool on 2d top view, (d) length of melt pool on the 2d top view, (e) mean value of temperature in melt pool domain, (f) maximum of peak temperature inside the melt pool border

Allied with the training of a RL agent in the FEM environment, Figure 100 (a-c) depict the achieved reward for the three agents (A1, A2, A3) and for the respective reward without control. The target of RL is increasing the summation of reward dynamically. By increasing the temperature in the melt pool, which is shown in Figure 106 (d, e), it is expected that the agent decreases the laser power. This behavior can be observed by agent A1, Figure 106 (a) where the reward remains at a crescendo throughout the episode but lower than the constant power. Agents A2 and A3 in Figure 106 (b, c), have a better reward than only the simulation with fixed power but, from step 30 on they have an erratic behavior as seen in the action graph in Figure 106 (b, c).

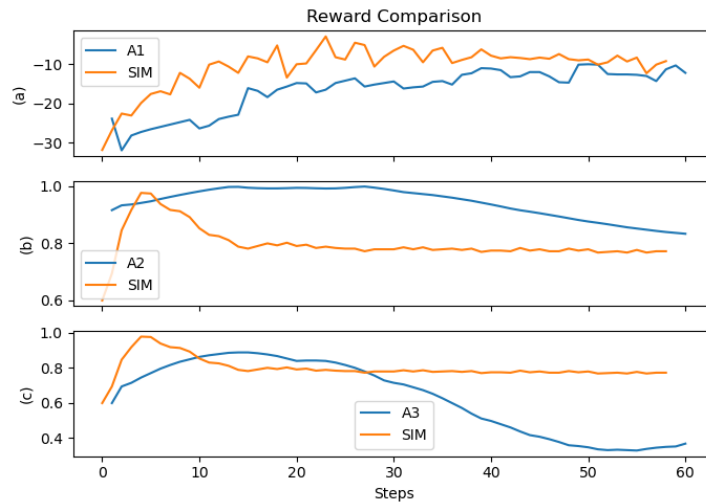


Figure 106 PPO performance with the reward representation during an evaluation episode for the three agents including (a) a1, (b) a2, (c) a3; and comparing with the simulation reward computed with the respective reward function

While the desired behavior is approaching, it is evident that additional training time is required to further refine the reward functions and the neural network policy. This approach demonstrates the potential of utilizing RL with OpenAI Gym for process control, particularly in a deliberate manner. By integrating it with the ABAQUS framework, we can initially train a model within a simulation environment, harnessing the capabilities of RL without incurring waste or utilizing machine time in real-world settings. This highlights the feasibility of leveraging RL for efficient and effective process optimization.

Chapter 8

Conclusion and future works

8.1. Conclusions

Additive manufacturing processes, such as Directed Energy Deposition (DED) and Powder Bed Fusion (PBF), hold immense potential for revolutionizing modern manufacturing. However, achieving optimal part quality and performance relies on a thorough understanding of the underlying thermal phenomena and microstructural evolution during the fabrication process. To address this challenge, a comprehensive computational framework is developed in this study to investigate transient heat phenomena in DED. The framework combines Finite Element Method (FEM) with a phase-field model, effectively tracking and capturing phase changes that occur during the deposition process. The model adeptly accounts for material transitions between molten, solid, and vaporized states, allocating appropriate thermal-physical material properties. Implemented within the renowned ABAQUS standard software, this model is easily accessible and adaptable for various applications in the field of Directed Energy Deposition. The validity and accuracy of the computational model are rigorously assessed by comparing simulation results of melt pool dimensions (width and depth) for single cladding lines with experimental data. The model's excellent agreement with the experimental results validates its reliability as a predictive tool for studying melt pool characteristics. Further exploration of the model's capabilities reveals intriguing insights into the effects of different laser power values on melt pool morphology. Higher laser power is found to lead to larger melt pool dimensions, indicating the strong influence of laser parameters on the deposition process outcomes. Additionally, a notable inverse correlation between scanning speed and melt pool volume emerges, with slower scanning speeds resulting in larger melt pools and faster speeds leading to smaller ones. This finding offers valuable guidance for optimizing processing conditions. The model also delves into the solidification process, accurately determining solidification parameters, such as temperature gradient (R) and growth rate (G). By leveraging temperature variation and the liquidus isotherm boundary surface information, the model effectively predicts the planar to dendrite transition, providing crucial insights into microstructural evolution during solidification. The study extends its scope to include thermal simulations of residual stress and distortion in both DED and PBF processes. Starting from cladding lines, the investigation progresses to single-layer and multi-layer structures. Consideration of critical factors, such as laser trajectory and dwell time, ensures accurate representations of deformation behavior. The study explores the relationship between residual stress and distortion in multi-layer structures, providing valuable understanding for process optimization.

Ultimately, this study aims to optimize the printing process parameters based on the simulation results, mitigating distortion and improving dimensional accuracy of printed parts. By addressing potential deformation issues caused by thermal loading, the study paves the way for practical

applications of additive manufacturing processes, particularly DED and PBF, in various industries.

In conclusion, the comprehensive computational models developed in this study offer valuable insights into the microstructural evolution and thermal behavior of materials during additive manufacturing. The findings contribute to the advancement of additive manufacturing techniques, guiding process optimization, and enhancing part quality for broader industrial applications. The brief list of conclusions can be found as follows:

- A computational framework for studying transient heat phenomena in the Directed Energy Deposition (DED) process has been successfully developed. The framework combines Finite Element Method (FEM) with a phase-field model, utilizing three state variables (ϕ_f , ϕ_v , and ψ) to accurately track and capture the phase of materials during the deposition process.
- The developed model accounts for the transition between different states of materials, including molten, solid, and vaporized states. It allocates appropriate thermal-physical material properties to accurately represent the behavior of materials under varying process conditions.
- The proposed model is implemented within the commercial finite element software ABAQUS standard, making it easily accessible and adaptable for different applications in the field of Directed Energy Deposition.
- To assess the capability of the numerical model, simulation results of melt pool dimensions (width and depth) for single cladding lines are compared with experimental data. The model demonstrates good agreement with the experimental results, validating its accuracy and reliability.
- The model is further used to investigate the effect of different laser power values on the melt pool morphology. The results indicate that higher laser power leads to larger melt pool width and depth, revealing the strong influence of laser power on the process outcomes.
- The numerical analysis also reveals an interesting inverse correlation between scanning speed and melt pool volume. Slower scanning speeds result in larger melt pools, while faster scanning speeds lead to smaller melt pools, providing valuable insights for process optimization.
- Solidification parameters, including temperature gradient (R) and growth rate (G), are effectively determined by utilizing temperature variation and the liquidus isotherm

boundary surface information. This information helps to understand the solidification behavior during the deposition process.

- The model predicts the planar to dendrite transition by moving from the melt pool boundary to the interior. This prediction aids in understanding the microstructural evolution and formation of dendritic structures during the solidification process.
- An inverse relationship between the temperature gradient (R) and growth rate (G) is observed, with maximum R near the top of the melt pool and minimum near the bottom. This finding is consistent with a solidification map obtained by scanning electron microscopy (SEM), further confirming the accuracy of the model's predictions.
- The cooling rate is found to increase from the bottom to the top of the melt pool. Additionally, decreasing laser power leads to an expanded range of the cooling rate, providing valuable information for controlling the cooling rates and resulting microstructures during the DED process.
- In the study, thermal simulations are employed to analyze the effects of direct energy deposition (DED) on residual stress and distortion in various structures, starting from cladding lines and extending to single-layer and multi-layer configurations. By utilizing thermal simulation results, we predict distortion during the DED process and gain a comprehensive understanding of thermal loading's impact on residual stress and distortion.
- The single-layer structures serve as a fundamental reference to calibrate material and process parameters, ensuring accuracy by comparing simulation results with experimental data. With this validation, we extend our analysis to multi-layer structures, enabling us to evaluate the cumulative effects of thermal loading throughout the printing process.
- Throughout the investigation, critical factors such as laser trajectory and dwell time are considered, as they significantly influence distortion. Consequently, simulation parameters are adjusted to account for these factors accurately.
- To deepen our understanding of the deformation behavior, we explore the relationship between residual stress and distortion in multi-layer structures. This comprehensive analysis allows us to identify key insights into the overall deformation behavior in additive manufacturing processes using DED.
- The ultimate goal is to optimize the printing process parameters based on the simulation results, mitigating distortion and enhancing the dimensional accuracy of printed parts. By doing so, we aim to provide valuable guidance for the design and optimization of additive manufacturing processes employing DED, addressing potential deformation issues caused by thermal loading. The insights gained from this study will contribute to

advancing the capabilities and reliability of DED technology for practical applications in various industries.

- The study focuses on investigating the characteristics of melt pools at the laser/powder interface in the Powder Bed Fusion (PBF) process using a phase-field thermomechanical model. To accurately model the physical phenomena during PBF, the finite element method is implemented within the MOOSE framework, incorporating the Adaptive Mesh Refinement (AMR) technique.
- The numerical model's performance is calibrated and assessed using the benchmark test of an optically-based metrological testbed (AMMT) provided by NIST. By comparing numerical temperature and phase change fields with experimental side track view observations, the model demonstrates acceptable agreement with measured melt pool dimensions.
- Moving on, the capabilities of the coupled model are evaluated on a three-dimensional PBF system, providing insights into temporal and phase changes during heating. The study explores the influence of the phase-field length parameter on temperature, melt pool geometry, and stress distributions, contributing to a deeper understanding of the process.
- Addressing the challenge of different thermal time scales at melting and solidification phases, the study utilizes MOOSE's automatic time scaling feature. This ensures accurate representation of the thermal behavior during different stages of the PBF process.
- Overall, the findings offer valuable insights into melt pool characteristics and the multi-physics aspects of the PBF process. This serves as a solid foundation for process optimization and enhancing the quality of manufactured parts.
- To expand future research, the study suggests exploring the "Stochastic Tools Module" within the MOOSE platform for surrogate modeling. This approach enables more efficient use of computational resources while capturing essential information.
- Furthermore, the study opens up opportunities for multi-layer simulations and digital twinning methods, with a consideration of computational limitations and constraints. By exploring these avenues, researchers can further advance their understanding of the PBF process and its potential applications.
- The study demonstrates the successful prediction of the microstructural evolution of metastable γ'' particles in a supersaturated γ matrix in the Ni-based superalloy, Inconel 625. This predictive capability is crucial for understanding the material's behavior and guiding its applications in various engineering scenarios.
- The morphological evolution and fractions of precipitate phases in a representative volume element (RVE) matrix are thoroughly investigated. This analysis provides

valuable insights into the hardening effects, which are essential for designing and optimizing additive manufacturing processes.

- A computational coupled phase-field model, skillfully developed using the MOOSE platform and finite element method (FEM), enables accurate simulations of the microstructural evolution. The combination of these powerful techniques proves to be effective in capturing the intricate behavior of precipitates in the alloy.
- The simulation's validity is verified by comparing the results with a benchmark for isothermal aging stages. This validation strengthens the confidence in the model's reliability and establishes its credibility for further analysis.
- The study examines the influence of alloy composition, lattice misfit, external stress, temperature, and time on microstructure and variant selection during non-isothermal heat fluctuations in additive manufacturing. This comprehensive exploration sheds light on the complex interplay of various factors affecting the material's evolution.
- An important aspect of the developed model is its ability to accurately predict precipitate formation without relying on predefined assumptions about size, shape, volume fraction, or spatial distribution. This remarkable feature enhances the model's versatility and applicability to diverse scenarios.
- The study particularly focuses on studying precipitation evolution under thermal cycles at two distinct points (A and B) in a 3D printed nickel-based superalloy. The analysis reveals the intricate effects of thermal cycles and oscillations on the formation of γ'' precipitates.
- At point A, the higher number of thermal cycles and more uniform heating/cooling conditions result in fewer but irregularly shaped nuclei during the first cycle. In contrast, point B experiences a higher temperature range and faster cooling, leading to a greater number of nuclei with more rounded shapes during the first cycle.
- The overall volumetric fraction of γ'' precipitates is found to be approximately 0.0481 for point A and 0.0983 for point B at 3670 seconds. These quantitative results provide valuable data for understanding the material's behavior and optimizing the additive manufacturing process to achieve desired microstructural outcomes.
- In conclusion, the study's comprehensive analysis and accurate predictions of microstructural evolution in the Ni-based superalloy, Inconel 625, offer valuable insights into material behavior under diverse conditions. The developed computational model, validated against benchmarks, exhibits great potential for guiding additive manufacturing processes and optimizing material properties for practical applications.

8.2.Future works

The integration of reinforcement learning (RL) techniques with the computational models and simulations developed in this study opens up promising avenues for further advancements in additive manufacturing processes. Building upon the comprehensive understanding of transient heat phenomena, microstructural evolution, and material behavior gained through the computational framework, the following future work proposes the creation of a clustered RL-based system for in-situ process correction and optimization.

- **Clustered RL Architecture:** A clustered RL architecture will be developed to efficiently correlate and analyze all the discovered features and parameters during the additive manufacturing process. The RL system will comprise multiple agents, each responsible for specific aspects of the process, such as laser power control, scanning speed adjustment, or thermal cycle optimization. This clustering approach will enable targeted optimization for different stages and components of the printing process.
- **Real-Time Sensing and Feedback:** To enable in-situ process correction, real-time sensing and feedback mechanisms will be integrated into the RL system. Sensors will continuously monitor key process variables, such as melt pool dimensions, temperature gradients, and cooling rates. The RL agents will receive this real-time data and make dynamic decisions to optimize the process parameters accordingly.
- **Objective Function Definition:** The RL system will be guided by an objective function that encompasses mechanical and process outcomes. Mechanical properties, such as tensile strength, hardness, and fatigue resistance, will serve as crucial performance indicators. The objective function will consider both quality metrics of the final product and energy efficiency to achieve environmentally sustainable manufacturing.
- **Exploration and Exploitation:** The RL agents will utilize a balance of exploration and exploitation strategies to optimize the additive manufacturing process. Initially, exploration will be emphasized to discover novel and promising process parameter combinations. Subsequently, exploitation will be employed to fine-tune the parameters based on past experiences and successes.
- **Continuous Learning:** The clustered RL system will engage in continuous learning through reinforcement and updates. As more data is collected during the additive manufacturing process, the RL agents will adapt their decision-making strategies to improve overall process performance and mechanical outcomes.
- **Multivariate Optimization:** The RL system will consider multivariate optimization, analyzing the interactions between different process parameters and their combined impact on the final product's mechanical properties. This approach will allow for holistic process optimization, considering all interrelated factors.

- **Calibration and Validation:** The RL system will be calibrated and validated against experimental data and benchmark tests to ensure its reliability and accuracy in achieving the best mechanical and process outcomes. The inclusion of physical experiments will provide valuable feedback for refining the RL-based process control strategies.
- **Scalability and Application:** The proposed RL-based system will be designed with scalability in mind, making it adaptable for different additive manufacturing technologies and materials. Its application will extend beyond specific case studies, enabling its deployment in diverse industrial settings.

In conclusion, the future work involves the development of a sophisticated clustered RL-based system that leverages the comprehensive computational framework and simulations to achieve in-situ process correction and optimization. By integrating real-time sensing, continuous learning, and multivariate optimization, this approach will enable additive manufacturing processes to achieve the best mechanical and process outcomes, advancing the capabilities and reliability of additive manufacturing technologies in various industries.

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