

A Robust Finite Element–AI Framework for Predicting Residual Stresses and Distortions in Laser Powder Bed Fusion Process

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Abstract

A Robust Finite Element–AI Framework for Predicting Residual Stresses and Distortions in Laser Powder Bed Fusion Process

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Metal additive manufacturing (AM), especially laser powder bed fusion (LPBF), enables the production of near-net-shape metallic components with complex internal features and part consolidation directly from digital designs, offering capabilities that are difficult or impossible to achieve with conventional manufacturing routes. LPBF is widely regarded as a cornerstone within digital manufacturing and the broader Industry 4.0 paradigm. However, despite its potential, LPBF still faces major challenges in producing defect-minimized structural components. Chief among these is the generation of high residual stresses, which can lead to excessive part distortion, crack initiation and propagation, and even structural failure. These issues arise from the highly localized and rapid heating and cooling cycles and associated phase transformations that occur during layer-by-layer melting and solidification process.

To address these challenges, the core objective of this research is the development of a high-fidelity, experimentally validated, multi-scale finite element (FE) modeling framework capable of accurately predicting residual stresses and distortions in LPBF-manufactured parts. A sequentially coupled thermo-mechanical simulation, based on the modified inherent strain (MIS) method, was implemented in Abaqus. In this framework, detailed thermo-mechanical simulations with a moving heat source and temperature-dependent material properties are first used to extract laser-induced thermal histories and applies the resulting thermal loads in the mechanical simulation to calculate modified inherent strains. These inherent strains are then fed into a reduced-order mechanical model to efficiently predict residual stresses and distortions. Several custom Python scripts, and user subroutines were developed for modeling phase transformations, hardening behavior, moving heat sources, and progressive element activation in Abaqus. To bridge the gap between microscale and macroscale modeling, a layer agglomeration technique was introduced,

allowing many physical layers to be represented by fewer equivalent computational layers, thereby reducing simulation time without compromising accuracy. Model validation was conducted using Inconel-718 cantilever beam samples in which various plasticity models including elastic-perfectly plastic, isotropic hardening, kinematic hardening, and Johnson-Cook, were evaluated and compared. The kinematic hardening model showed the best agreement with experimental results, with less than 6% deviation and significantly improved computational efficiency. Additionally, the MIS model's capability to predict subsurface residual stresses was evaluated using cube coupons made of Inconel-625, addressing a critical gap in the existing literature.

To further accelerate the simulation process, a machine learning (ML) model was trained using data from the developed high-fidelity models to predict inherent strains directly from process parameters. The ML model could estimate the strains with an average relative error of 18% for three material types compared to FE results. When embedded in the FE framework, this hybrid ML–FE approach reduces computational cost by up to four orders of magnitude ($\sim 10,000\times$) while maintaining reliable accuracy, with residual stress and distortion predictions within 16% of the high-fidelity reference solutions.

Overall, this work provides a robust, scalable framework for predictive modeling and process optimization in LPBF, paving the way toward reliable, reduced-distortion AM production.

Dedication

To my loving wife, Ilda, for your unconditional love, understanding, and patience. Your unwavering support has been the rock on which I built my dreams.

And

To my beloved mother, Zahra, and the eternal soul of my dear father, Nader, and my sympathetic sister, Neda, whose boundless love, support, encouragement, and blessings have been my guiding light through every step.

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Contribution of Authors

This thesis is written in a manuscript-based format. Chapters 1 and 6 are the introduction and conclusions of the thesis, respectively. The thesis includes co-authored works in Chapters 2, 3, 4, and 5 that were reprinted from papers published or submitted to scientific journals. The contribution of each co-author is described below:

Chapter 2:

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Hossein Mohammadtaheri worked on the critical review article and performed the material preparation, data collection, and analysis. All authors contributed to the study conception and design. The first draft of the manuscript was written by Hossein Mohammadtaheri, and all authors commented on previous versions of the manuscript. R. Sedaghati and M. Molavi-Zarandi supervised the research and reviewed and revised the manuscript.

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Hossein Mohammadtaheri conducted the literature review and developed the methodology. He performed the finite element numerical simulations, collected and analyzed the data, validated the results through experiments, discussed the findings, drafted the original manuscript, and contributed to its review and editing. R. Sedaghati and M. Molavi-Zarandi supervised the research and contributed to the review and revision of the manuscript.

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Chapter 5:

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Chapter 1 Introduction

1.1 Introduction

In the realm of metal additive manufacturing (AM), laser powder bed fusion (LPBF) is one of the most widely used techniques for producing complex metallic components. The LPBF involves melting and fusing layers of metal powder with a focused laser heat source that follows a predetermined scanning pattern, building up a 3D part layer by layer through repeated deposition and solidification. As a result of the intense laser power focused on a small area and the locally high energy density, a significant spatial and temporal temperature gradients develop. This leads to phase transformations and rapid heating and cooling cycles, which cause the generation of substantial residual stresses and subsequent distortions in the fabricated components [1,2].

The significance of residual stress and distortion in the context of design and optimization has spurred extensive research into various methods for quantifying and predicting these factors in components produced by the LPBF process. While experimental exploration remains essential for understanding the intricate physics of the process, the cost and time associated with such experiments have led researchers to increasingly turn to thermo-mechanical simulations which can explicitly illustrate the spatial and temporal evolution of temperature, thermal stresses, and distortions. Typically, when it comes to the fidelity of conceptual frameworks for simulating the LPBF process, they are categorized into microscale, mesoscale, and macroscale (part-scale) models [3,4]. The microscale models delve into micron-level fluid dynamics within molten pools and the development of microstructures [5–7]. Conversely, the mesoscale and macroscale models simplify the detailed melt pool fluid flow and solidification mechanisms to ensure computationally efficient analysis and therefore do not explicitly resolve many of these fine-scale physical phenomena. For example, Goldak's double ellipsoidal and Gaussian models are commonly used in the mesoscale simulations to approximate the laser as an equivalent moving volumetric heat source, enabling the evaluation of temperature, stress, and strain profiles via a coupled thermo-mechanical analysis [3].

Detailed coupled thermo-mechanical simulations [8–10] enable a comprehensive and accurate assessment of residual stress and distortion using moving heat source models [11–13]. However, this approach proves inefficient for predicting part-scale outcomes due to prohibitive computational costs [14]. Hence, to address the significant computational workload, several investigations have been undertaken to examine the inherent strain (IS) method introduced by Ueda [15,16] as a practical and efficient approach for predicting residual stress in welded components. Moreover, a plastic strain method, inspired by the inherent strain theory, was formulated to calculate the residual distortion in the laser-engineered net shaping process [17,18]. Both of the proposed methodologies have been shown to result in a substantial reduction in computation time. Given the similarities between numerical simulations of the LPBF and multi-pass welding processes, there has been a notable interest in extending the applicability of the IS method to AM components [19]. Comprehensive investigations into this possibility have demonstrated that implementing this well-established method in AM can significantly reduce computational costs. This can reduce the analysis duration from weeks or months to a mere few days or hours, all while preserving accuracy in comparison to detailed thermo-mechanical simulations [20–23].

In summary, the IS method offers an efficient approach to incorporate scanning strategies into LPBF simulations while significantly reducing computational demands. Rather than modeling the real-time thermal input, this technique effectively utilizes precomputed strain fields derived from mesoscale or detailed local analyses. These inherent strain fields, which reflect the influence of the thermal history through various scanning strategies, are subsequently applied to a macroscale FE model. This approach streamlines the simulation process, allowing for the prediction of residual stresses and distortions across the entire component without the intensive computation required by conventional thermo-mechanical simulations.

Despite significant advancements in IS-based simulation technique over the past decade [24–29], important limitations still remain. Most existing IS-based LPBF studies neglect the influence of strain hardening and strain-rate sensitivity in the plastic constitutive response, potentially limiting accuracy in high-gradient and cyclic thermal environments inherent in LPBF process [27,30,31]. Depth-resolved (subsurface) residual stress distributions in LPBF components have also received limited attention, despite their relevance to crack initiation and fatigue performance. Furthermore,

very limited studies have explored the integration of IS frameworks with machine learning (ML) to efficiently map process parameters to inherent strains and subsequently resulting residual stresses and distortions. Addressing these limitations calls for high-fidelity yet computationally efficient prediction frameworks that combine inherent-strain-based FE models with data-driven meta-models. These research gaps have motivated the research objectives outlined in Section 1.2.

1.2 Research Objectives

The IS-based methods emerge as a rather novel thermo-mechanical modelling approach for predicting induced residual stresses and distortions throughout the part manufactured by the LPBF process. Nevertheless, there remain key gaps that must be addressed to fully exploit their potential:

- Most previous IS-based LPBF studies neglect the effect of strain hardening and rate of hardening in plastic yielding law;
- No prior work has specifically addressed the characterization of residual stress distribution within the subsurface region;
- Very limited studies on the integration of IS framework with ML to account for the effect of different process parameters on the induced residual stresses and distortions.

Motivated by these gaps, the main objectives of this research study respecting the sequence of the chapters of this thesis are outlined as below:

- **Development of a multi-scale thermo-mechanical FE model:** Development of a multi-scale and high-fidelity thermo-mechanical FE model to accurately predict the temperature history and induced residual stresses and distortions through the LPBF process. The numerical model is based on the concept of the IS method. Temperature-dependent material properties, as well as the influence of hardening and rate of hardening, are incorporated into the model.
- **Experimental and numerical validation of induced residual stresses:** Conduct a detailed investigation of residual stress distribution along the depth of LPBF-manufactured parts and validate the numerical predictions against experimental measurements. This depth-resolved comparison offers new insights into subsurface stress evolution in LPBF components and addresses a significant gap in literature.

- **Development of a hybrid FE-ML model to predict inherent strains:** Development of an advanced AI model that incorporates the IS-based approach to efficiently estimate the inherent strains for specific process parameters and material properties without performing detailed mechanical simulation at mesoscale. This hybrid FE–ML approach accelerates the prediction of residual stresses and consequently distortions for part-scale components and enables more efficient process design and optimization.

To achieve the first objective, Inconel-718 for the printed cantilever beam is analyzed, whereas for the second objective, Inconel-625 with a cube coupon geometry is examined. This systematic choice of different material systems and geometric configurations enables assessment of the robustness and accuracy of the proposed modelling framework across multiple LPBF applications and scales.

1.3 Thesis Organization

This thesis comprises six chapters. Each chapter is briefly described herein.

Chapter 1 (Introduction)

This chapter introduces the LPBF process and its key physical mechanisms. It highlights the importance of the LPBF process simulation for predicting residual stresses and distortions, and the efficiency of the IS method over the detailed thermo-mechanical approach, followed by the research gaps and objectives addressed in this thesis.

Chapter 2 (Paper 1)

This chapter provides a critical literature review of inherent strain–based modelling for LPBF and related thermal processes. It emphasizes methodological developments, summarizes the main achievements and limitations of recent studies, and identifies opportunities for improving IS-based frameworks, particularly in terms of accuracy, constitutive modelling, and computational efficiency.

Chapter 3 (Paper 2)

This chapter represents the impact of hardening on the prediction of residual stresses and distortions in Inconel-718 for IS-based LPBF simulation. Different plastic constitutive models are compared, and their influence on predicted residual stress fields and part deformation is quantified and discussed.

Chapter 4 (Paper 3)

This chapter presents a detailed evaluation of the modified IS method using combined numerical and experimental studies on LPBF-manufactured components. Depth-resolved residual stress measurements are used to validate the MIS framework, and key insights are drawn to guide future improvements in residual stress prediction for LPBF parts.

Chapter 5 (Paper 4)

This chapter presents a novel data-driven approach combined with FE modeling to enhance computational efficiency in the non-linear coupled thermo-mechanical simulations. The proposed hybrid FE–ML framework accelerates the prediction of residual stresses and, consequently, distortions for part-scale LPBF components while maintaining acceptable accuracy.

Chapter 6 (Conclusion and Future Work)

This chapter summarizes the main findings, contributions , and limitations of the research. It emphasizes the major achievements and underscores the importance of the findings. Furthermore, it identifies promising directions for future research and offers suggestions to support continued progress in the field.

Chapter 2 Inherent strain approach to estimate residual stress and deformation in the laser powder bed fusion process for metal additive manufacturing - A state-of-the-art review

Abstract: In recent years, metal additive manufacturing (AM) and particularly the laser powder bed fusion (LPBF) process has substantially grown in popularity in industrial applications due to its unique ability to produce a wide variety of components with complex geometry. The LPBF process is now an integral part of digital manufacturing and the industry 4.0 concept. However, a considerable amount of residual stress and deformation induced by the fast and intense heating/cooling cycle as well as phase change in each layer are still some important technical barriers in the LPBF process, giving rise to increasing inaccuracy and structural failure in some cases. Developing an efficient physics-based simulation model capable of predicting the induced residual stresses is, thus, of paramount importance to build parts with minimal distortion in a wide range of applications, while avoiding expensive and time-consuming experimental procedures. The simulation model also is efficiently utilized to investigate the effect of process parameters, material, and geometry on the development and redesign of parts. In the last decade, multi-scale process modeling frameworks have been developed to predict residual stress and deformation cost-effectively in the parts fabricated by LPBF. The purpose of this survey is to systematically provide an in-depth overview of the inherent strain modeling approach with a focus more on the methodology development, highlighting the positive outcomes and limitations of recent investigations, followed by presenting potential future work to optimize this technique.

2.1 Introduction

In the past decade, the versatile metal laser powder bed fusion (LPBF) has been recognized as an accepted method for the fabrication of complex-shaped prototypes with excellent resolution, high performance, reduced material waste, and dramatically shortened time between design and manufacture [32,33]. Despite these superior properties, many applications in the biomedical, aerospace, and automotive industries are affected by several restrictions and technical barriers, ranging from porosity defects, micro-cracks, and balling effect to warping and distortion related to large temperature gradients experienced in the LPBF process [7,34–38]. Typically, the LPBF

utilizes a high-density laser beam as a thermal source to selectively melt the materials in the form of powder onto a build plate along a pre-defined scanning route in a layer upon layer fashion. Deposited layers are fused together based on the sliced layer geometry until the desired shape is entirely built. Due to a high magnitude of temperature gradient, phase change transformation, and fast thermal and cooling cycles, a significant amount of residual stress is created, and subsequent deformation occurs in the components [1,2,30]. Although many experimental investigations using X-ray diffraction, hole drilling, contour method, and laser line profilometry have been conducted to study the influence of different process parameters on residual stress formation [39–48], these experiments are not only often very costly and time-consuming, but they cannot also explicitly demonstrate how the temperature and thermal stress fields evolve over time. For instance, Kantzos et. al [49] examined the effects of beam power, scan speed, and hatch spacing alterations on the microstructures and mechanical properties of Inconel 718. Zachary et al. [50] determined the characteristics and propagation mechanisms of five principal forms of spatter during the LPBF process by using in-situ high-speed, high-energy X-ray imaging. Gockel et al. [51] proposed a method to determine the relationship between surface roughness and laser power and speed and fatigue performance of alloy 718. Nayak et al. [52] successfully achieved the LPBF of a dense IN625 at a higher layer thickness of 100 μm by varying the combined parameters of laser energy density. Obviously, the LPBF process is affected by several contributing factors, such as material types, process parameters, and the geometry of the part. The examination of the effect of these factors on the induced thermo-mechanical residual stresses and distortion experimentally would be impractical if not impossible. Although experimental validation is still necessary, a reliable numerical modelling may significantly reduce the number of costly experimental trials in some certain conditions. Therefore, numerical-based techniques have emerged as promising tools to fundamentally understand the multiple highly coupled thermophysical phenomenon occurring during the LPBF process and to systematically investigate the effect of process parameters, material, and geometry factors on the induced residual stresses and part defects. The validated high fidelity numerical simulation model can be effectively utilized to accurately and efficiently predict the temperature distribution, induced residual stresses, and distortion in the entire parts under varied process parameters and part's geometry and material factors without carrying out time-consuming and expensive trial and error experiments.

In the LPBF process modeling, a significant amount of computational effort is required due to highly non-linear plastic deformation, transient heat transfer, fluid dynamics, and chemical reactions within the melt pool [53]. One of the major challenging issues in the simulation and modeling of LPBF is taking into consideration all complex multi-physics namely, phase change transformation from solid to liquid, wetting and capillary forces, Marangoni convection phenomenon, recoil pressure, surface tension, and vaporization [54]. As a result, considering all the complex multi-physics in modeling leads to increasing computational time significantly for solving the problem. Because fluid dynamics equations and chemical reactions have negligible effects, they are frequently ignored in many studies focusing on residual stress and deformation prediction [55,56]. Induced residual stresses and deformation have been initially predicted by the detailed thermomechanical simulations using a thermal source model [8–10,57–61]. However, despite its high accuracy, due to an infinitesimal laser spot size and thousands of thin layers with a thickness at the micron level, the LPBF detailed thermo-mechanical simulation for the complex geometric parts requires a large number of time steps to estimate residual stress and deformation, which is not computationally cost-effective. Furthermore, based on the large thermal gradient near the heat source, the mesh size must be sufficiently small to accurately predict the induced residual stress and deformation of the deposited layers in the heat affected zone. Therefore, applying a coupled thermo-mechanical analysis for multiple laser scans with a fine mesh model to macro-scale simulation would incur excessively large computational costs. Additionally, the large number of degrees of freedom for each element in the mechanical analysis leads to higher complexity as well as a longer amount of processing time. Detailed thermo-mechanical analysis for an industrial component is almost impractical since it would demand hundreds of terabytes of memory and years to calculate. Although many simplified strategies, such as the layer lumping method [62–65], static and dynamic adaptive mesh refinement techniques [59,66–71], multi-scale modeling framework [37,62,65], and simplified heat source modeling and heat transfer problems [20,72], have been developed over years to improve the efficiency of LPBF simulation with reasonable accuracy, the computational time has not been significantly improved, particularly for complicated industrial components. To overcome the huge computational burden associated with the numerical simulation of LPBF process, a number of studies have been conducted to explore the inherent strain method (ISM) proposed by Ueda [15,16] as the most viable and efficient approach to predict the induced residual stress in the welded parts. Furthermore, the applied plastic strain method

inspired by the inherent strain theory was developed to predict the residual distortion of laser engineered net shaping process [17,18]. Both the suggested methods led to reducing the calculation time significantly. Since the numerical simulation of PBF is almost similar to the multi-pass welding process, the extension of the ISM in AM parts was drawn remarkable interest [19]. The possibility of applying this well-established method in AM was comprehensively investigated, demonstrating that the computational cost may be decreased from potentially days or weeks to a few hours while maintaining the accuracy compared to the detailed thermo-mechanical simulation [20–22]. Although the ISM has been introduced in many commercial software packages such as Abaqus [73,74], MSC Simufact [30], Autodesk Netfabb [69], and Ansys [74,75] for industrial parts simulation, their underlying algorithms (i.e. how the inherent strains are extracted and applied to the part-scale model) are not described in detail.

This paper attempts to provide a comprehensive overview of finite element-based modeling of the LPBF process using the inherent strain approach. In section 2.2, an explanation of fully and partially coupled thermo-mechanical simulation involving their governing equations is presented. Furthermore, it summarizes the articles that discussed the classical inherent strain theory, based on the physical phenomenon in the welding process. In section 2.3, a detailed description of thermal and mechanical simulations at the multi-scale framework using the modified inherent strain method (MISM) is presented. In section 2.4, the practical implications of the research associated with the ISM are reviewed. Finally, the conclusion and some future research possibilities are provided.

2.2 Thermo-mechanical simulations

The detailed thermo-mechanical simulation is divided into fully coupled and partially coupled techniques. The fully coupled method considers the thermal and mechanical analyses consecutively in which the temperature field is affected by modified geometry in every increment. The partially coupled method, on the other hand, utilizes the temperature history derived from a complete transient thermal analysis as a thermal load to be used in structural analysis separately [76]. Due to the poor coupling between the mechanical and thermal fields in the LPBF process and also computational efficiency, the majority of research studies are based on the partially coupled approach [1]. In this section, the governing equations for the detailed thermo-mechanical simulations are provided in order to have a better understanding of their differences and

implementation of the finite element method based on these approaches. In addition, following the explanation of the classical inherent strain theory as an efficient alternative numerical method in welding and AM simulations, some of the associated improvements and validations are discussed.

2.2.1 Fully coupled approach

The typical flow chart for the fully coupled modeling of temperature and thermal stress fields in the LPBF process is illustrated in Fig 2.1 [77]. The coupled temperature-displacement analysis is performed sequentially from the bottom layer to the final top layer, wherein each layer, it is conducted on every increment of each scanning track. In the early stage of the analysis, which is done on the first scanning track of the substrate, since the displacement is zero, the temperature field extracted from the thermal analysis in the first increment is applied as a load to determine the displacement value for the next increment. This procedure continues increment by increment from each layer to another layer, until the last increment in the final scanning track of the top layer is being analyzed. As a consequence, the residual stress and deformation of the built part can be predicted.

The governing heat transfer energy equation of coupled thermoelectricity for temperature distribution can be written as follows [78]:

$$kT_{,ii} - \rho c \dot{T} - \alpha T_0 (3\lambda + 2\mu) \dot{\epsilon}_{ii} + Q = 0 \quad (\text{Eq 2.1})$$

where ρ is the material density, c is the temperature-dependent heat capacity, T is the temperature, k is the temperature-dependent thermal conductivity of the material, λ and μ are the Lamé elastic constants, α is the coefficient of thermal expansion, T_0 is the reference temperature, ϵ is the strain, and Q rate is defined by the heat generated within the body per unit volume and unit time. As can be seen in the fully coupled approach, the governing transient heat transfer equation for temperature variation includes the rate of strain.

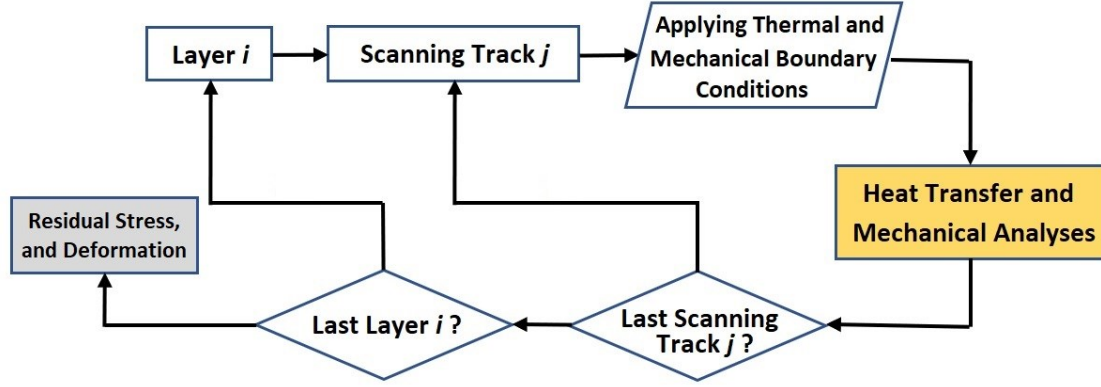


Fig 2.1 Flowchart of fully coupled thermo-mechanical FE model [77]

The governing equation for displacement can be derived by combining the equations of motion, strain-displacement relations and constitutive Hook's law equation stated as, [78,79]:

$$\text{Equations of motion: } \sigma_{ij,j} = \rho \ddot{u}_i \quad (\text{Eq 2.2})$$

$$\text{Strain-displacement relations: } \epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \quad (\text{Eq 2.3})$$

$$\text{Constitutive equations: } \sigma_{ij} = 2\mu\epsilon_{ij} + \lambda\epsilon_{kk}\delta_{ij} - (3\lambda + 2\mu)\alpha(T - T_0)\delta_{ij} \quad (\text{Eq 2.4})$$

Substituting Eq 2.3 for strains into Eq 2.4 and then substituting the resultant into Eq 2.2 yields the following governing equation for displacement:

$$\mu \nabla^2 u_i + (\lambda + \mu) u_{k,ki} - \alpha(3\lambda + 2\mu)(T - T_0)_{,i} + F_i = 0 \quad (\text{Eq 2.5})$$

where F_i is the body force per unit volume and δ_{ij} denotes the Kronecker's symbol expressed by:

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \quad (\text{Eq 2.6})$$

Eqs 2.1 and 2.5 are fully coupled with respect to both temperature and displacement. These coupled equations together with initial and boundary conditions for thermal and mechanical loads can provide the displacement and temperature distribution in a part.

2.2.2 Partially coupled approach

In the partially coupled simulation, a thorough thermal analysis for the given geometry and boundary conditions is performed first, and the resultant temperature history is implemented as thermal loads in the quasi-static mechanical analysis. Therefore, the thermal and mechanical

governing equations are independent (Fig 2.2). The energy Eq 2.1 is simplified to a 3D heat transfer Fourier equation for homogeneous isotropic materials to obtain the transient temperature distribution as follows:

$$kT_{,ii} - \rho c \dot{T} + Q = 0 \quad (\text{Eq 2.7})$$

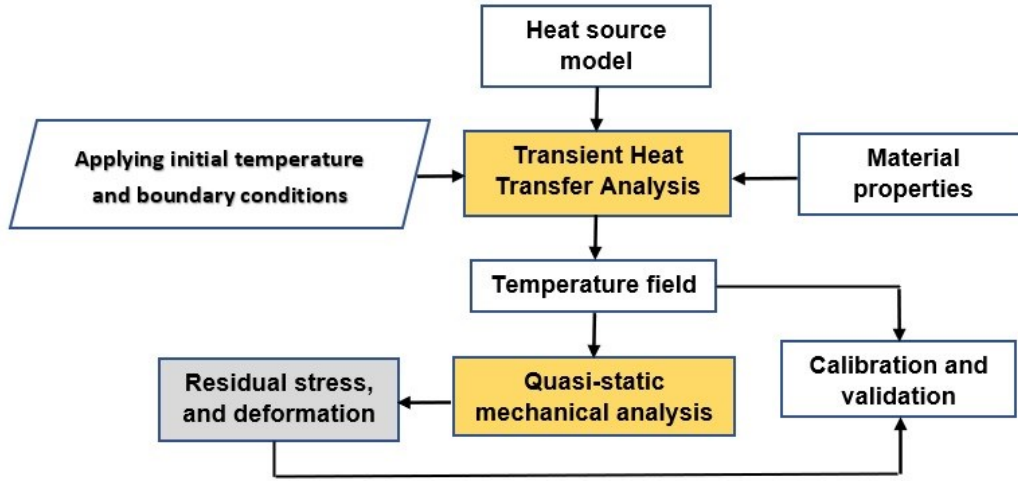


Fig 2.2 Flowchart of partially coupled thermo-mechanical FE model

In mechanical analysis, the material constitutive model can be assumed to be either elastic and perfectly plastic with the $J2$ -von Mises plasticity law [30,80] or pure plastic behavior with isotropic/ kinematic or mixed strain hardening rules, using the associative $J2$ plasticity law [81,82].

$$\sigma = C : \varepsilon_e \quad (\text{Eq 2.8})$$

$$\varepsilon_{total} = \varepsilon_e + \varepsilon_p + \varepsilon_{th} \quad (\text{Eq 2.9})$$

$$\varepsilon_{th} = \alpha \cdot \Delta T \quad (\text{Eq 2.10})$$

$$f_{yield} = \sigma_m - \sigma_Y = 0 \quad (\text{Eq 2.11})$$

where C is the fourth-order material stiffness tensor, ε_e , ε_p , ε_{th} are the second-order elastic, plastic, and thermal strain tensors, respectively, α is the temperature-dependent coefficients of thermal expansion and ΔT represents the temperature change during the process. σ_m is the von Mises's stress, and σ_Y is the yield stress determined by the uniaxial tensile test. To consider the strain hardening rules, σ_Y can also be expressed by the Johnson-Cook plasticity model [83]. Typically, it is assumed that plastic strain occurs for $f_{yield} > 0$.

2.2.3 Original Inherent Strain Method (ISM)

Based on the proposed method by Ueda [15,16], the inherent strain method involves two main steps: 1) Conducting a detailed thermo-mechanical simulation on a microscale specimen to compute the plastic strain tensor once the built part cools down to room temperature; 2) Applying the resultant plastic strain tensor to an actual component and performing a linear elastic analysis. In computational welding mechanics, the micro-welding process involves rapid heating, melting, and cooling cycles of the material along the weld line, which results in a significant temperature gradient and residual deformation [23]. Therefore, the total strain throughout the process is constituted by the summation of elastic, plastic, thermal, and phase change strains. The original inherent strain theory assumes that the total elastic strain is relieved after the welded part is cooled down to ambient temperature. Moreover, considering the final cooled state of the part, the thermal strain vanishes. Thus, by neglecting the infinitesimal phase change strain for the simplification [16], the inherent strain equals the plastic strain formed during the welding process.

Keller and Ploshikhin [21] applied the inherent strain theory in a new multi-scale approach to the AM process for the first time to approximate the deformation and residual stress distribution. They proposed three models at different lengths and time scales to account for both thermal and mechanical development during the LPBF process, namely microscale calibration of a heat source model, mesoscale analysis of the hatching strategy to extract the inherent strains, and macroscale development of a mechanical layer equivalent (MLE) model. The small-scale modeling includes laser power, scanning speed, hatching pattern, and layer thickness as the main process parameters. The computed inherent strains obtained from the mesoscale are then loaded onto a macroscale finite element model as the initial strains to predict the residual stress and deformation by a linear elastic analysis. This multi-scale framework based on inherent strain approach to predict the residual stress and deformation in LPBF process are clearly shown in Fig 2.3. The element activation methods [84,85] are used in both the detailed process and part-scale modeling to accelerate the numerical simulation. Their findings were very well matched with experimental results, and the method was shown to be more computationally practical than conventional thermo-mechanical simulations.

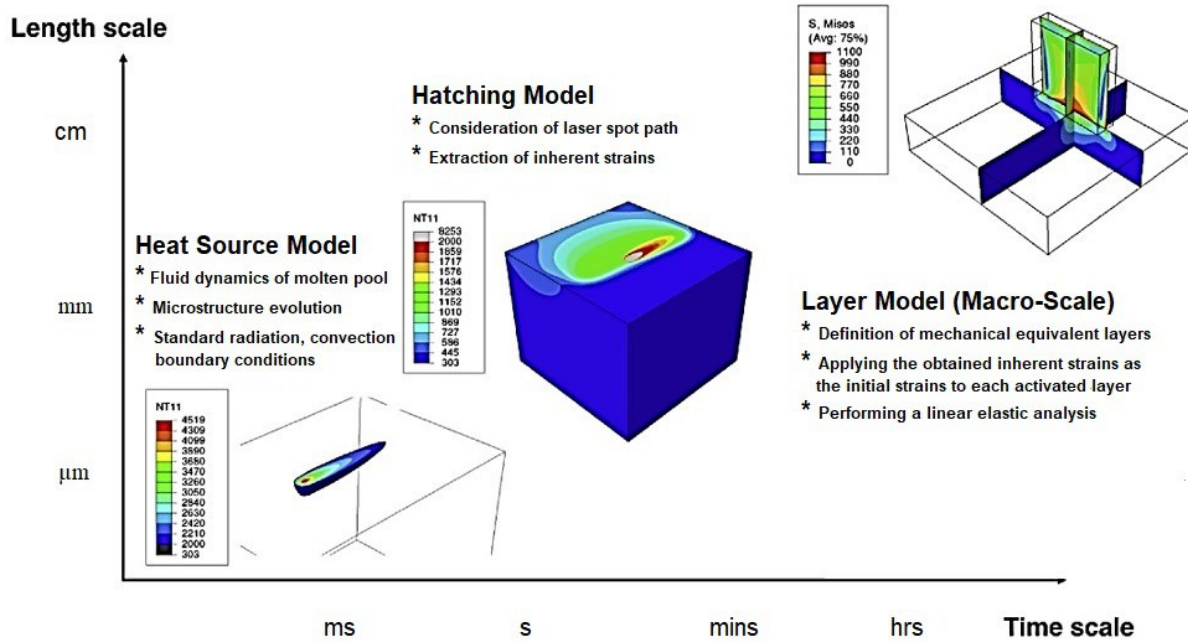


Fig 2.3 Multi-scale framework using inherent strain approach to predict residual stress and deformation in LPBF [80]

Following the proof of the inherent strain method's suitability to the AM process, further studies were conducted in order to enhance this breakthrough. Bugatti and Semeraro [22] investigated the limitations of the inherent strain method (ISM) in the LPBF process both numerically and experimentally. They indicated that the macroscopic dimensional features had an influence on the inherent strain in their experiments, which implies that the basic geometry-independence assumption of inherent strain in the previous studies may be problematic. As a result, the ISM must be calibrated as the geometry becomes more complicated. Siewert et al. [24] delved deeper into the mechanical layer equivalent model by using the inherent strains obtained from experimental calibration in two cantilever beams fabricated by LPBF. Their numerical model accurately predicted residual deformation based on experimental results. Ahmad et al. [25] indicated the consistency between the residual stress values estimated by inherent strain and contour methods. It was found that the formation of tensile and compressive residual stresses occurs near the surface (along the edges) and at the center area of samples, respectively. Furthermore, Setien et al. [26] presented an empirical methodology to determine inherent strains based on classical laminate theory (CLT) in composite laminates. They established a strong correlation between the sequential layer-wise LPBF process, and the technology utilized to fabricate composite laminates. Considering the same effects of the hatching sequence and fiber orientation, the unique inherent

strains that correspond to each layer are determined by iteratively optimizing the discrepancy between estimated residual distortions and experimental results of twin cantilever beams (Fig 2.4). As a key finding of their research, the inter-layer inherent strains tend to be consistent when the laser scanning route turns regularly regardless of rotational angle. However, despite its good accuracy, the need for numerical optimization and the fabrication of a large number of samples restrict the use of this costly methodology in industry.

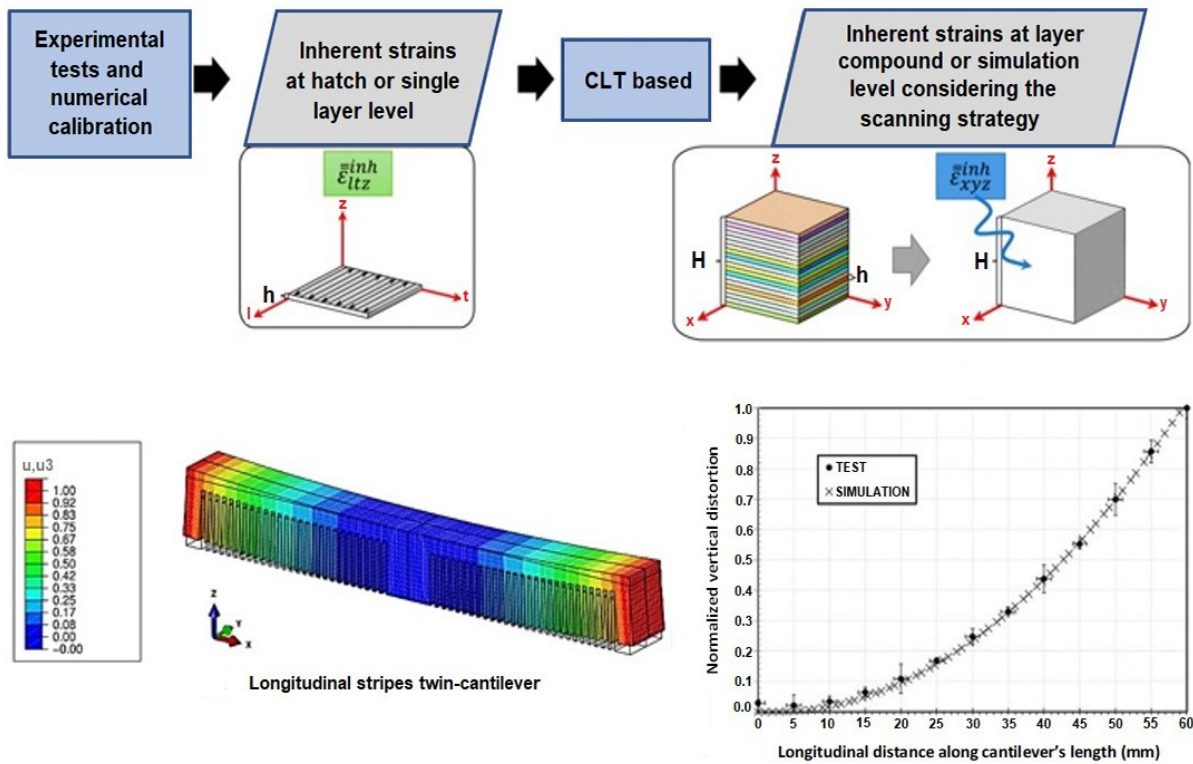


Fig 2.4 Inherent strain determination strategy based on experimental tests for double cantilever beam [26]

2.3 Modified Inherent Strain Method (MISM)

2.3.1 Concept of MISM

The original inherent strain theory made the key assumption in the microscale simulation that the elastic strain is negligible in comparison to the plastic strain after the part is cooled down to room temperature. However, due to the difference between the physical phenomena of LPBF and the welding process resulting from the fast-moving heat source and multi-layer build model, this hypothesis cannot be employed in the LPBF process. Theoretically, throughout the LPBF, mechanical boundaries evolve with melting and solidification when additional layers are deposited, reaching a steady-state after printing subsequent layers. Thus, the elastic strain cannot

be fully relieved when the part cools to ambient temperature [23]. The concept of the modified inherent strain method (MISM) was basically formulated by considering the contribution of two main factors during the process as follows:

$$\varepsilon^{In} = \varepsilon_{plastic}^I + (\varepsilon_{elastic}^I - \varepsilon_{elastic}^S) \quad (\text{Eq 2.12})$$

where I and S represent the period of time belonging to the intermediate and steady-state conditions, respectively. In the modified version, the inherent strains taken from the mesoscale are implemented into the macroscale as the constant coefficients of thermal expansion in x , y , and z directions, and a unit temperature increase is applied to each activated layer. Due to the much smaller value of the shear strains than the normal strains, the inherent shear strains are neglected in the multi-scale framework without sacrificing precision [23].

The mechanism of intermediate and steady states can be explained by the temperature and strain evolution of a bottom layer (first layer) in a 3-layer simulation through the MISM as illustrated in Fig 2.5 [30]. Fig 2.5(a) represents the formation of compressive elastic and plastic strains at the early stage, as the material powder is sintered, which later transforms into tensile strain caused by further printed layers. The three sequential temperature peaks in Fig 2.5(b) reflect the thermal history of the first deposited layer, with the second and third peaks resulting from succeeding layer depositions. According to Eq. (12), two significant sources are considered in the modified inherent strain theory: 1) the contribution from compressive plastic strain at the intermediate state and 2) the influence of thermal shrinkage coupled with the inter-layer effect. The accumulation of initially compressive strain in the intermediate state is due to a substantial drop in mechanical strength at an elevated temperature where the non-uniform thermal expansion, induced by a sharp temperature gradient in the melt pool area, is restrained by neighboring solidified metals. When the component is cooled to room temperature, the magnitude of compressive stress and strain is reduced, becoming tensile as a result of thermal contraction. Regarding the steady-state, Fig 2.5(c) and (d) depict the significant relief of elastic strain by thermal shrinkage of surrounding solidified materials and previously deposited layers, demonstrating the small and profound impact of subsequent depositions on the plastic and elastic strain of the first layer, respectively. In the following sections, some groundbreaking research on MISM has been systematically reviewed.

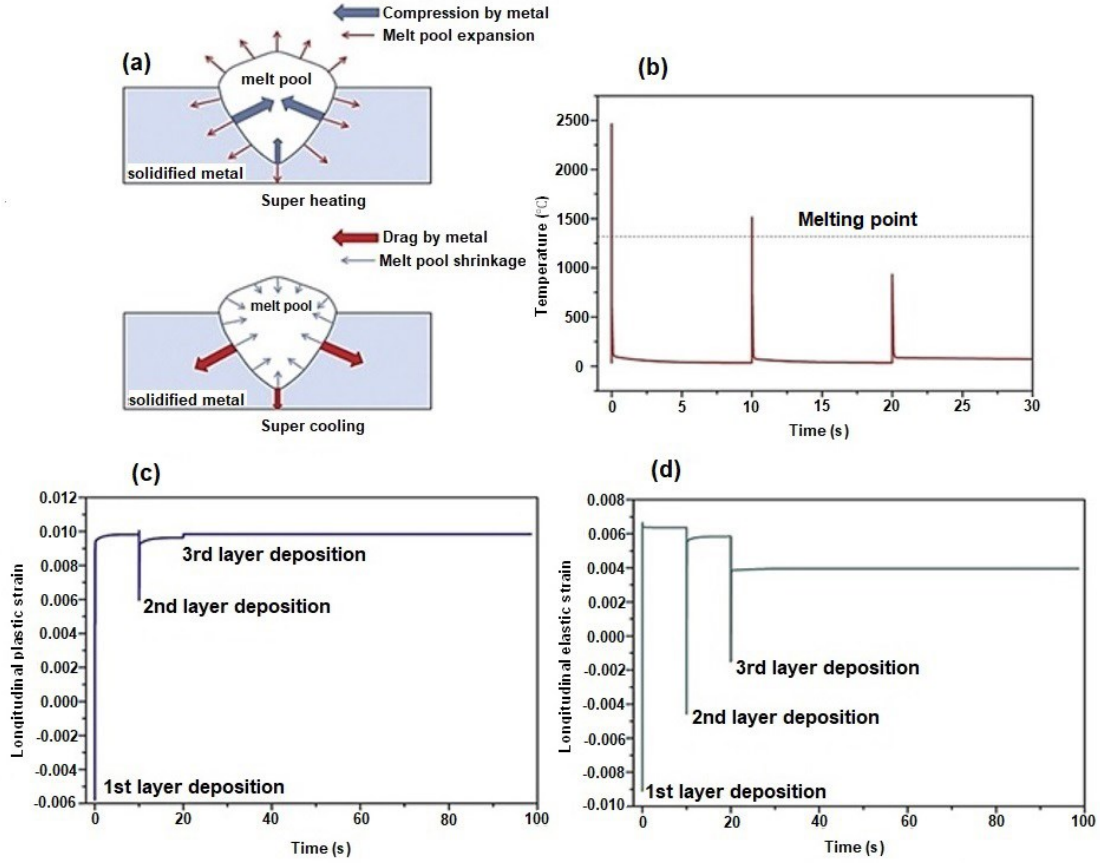


Fig 2.5 (a) Mechanism of compressive and tensile strain; Bottom layer (b) Thermal history, (c) Plastic strain and (d) Elastic strain evolution history [30]

2.3.2 Validation and layer lumping effect

Several recent studies have confirmed the validity and efficiency of the MISM when applied to the LPBF process. For instance, Chen et al. [30] estimated the deformation of a double cantilever beam and a complex canonical part by the MISM in LPBF process, which was in close agreement with experiments. They proved that the microscale modeling of a 2-layer and 3-layer can nearly capture the same results due to the limited impact of the third deposition on the strain evolution of the bottom layer. Furthermore, in another research study [27], they demonstrated that the residual deformation accuracy can be improved by more than 20% when using the MISM compared to the original inherent strain method in a double cantilever beam simulation. Moreover, according to the equivalent layer model in MISM, when a number of physical layers are lumped into one equivalent layer and a unit temperature rise is adopted to the equivalent layer in a load step, a particular number of lumped layers must be determined to accelerate the non-linear layer-by-layer simulation while ensuring accurate predictions. Their findings revealed that a thinner thickness of the

activation layer (i.e. less layer lumping) would cause an underestimation of residual stress and deformation. The most plausible reason behind this phenomenon is that the tensile stress is generated in previous depositions due to the mechanical constraints induced by lower layers, and the thermal shrinkage of new deposited layers contributes to the shrinkage of already deposited layers, resulting in an underestimation of tensile stress in lower layers due to the stress relief effect. Based on some simple numerical trials, the feasible layer activation thickness was identified as being between 0.4–0.6 mm for different cases [27]. However, the successive layer-by-layer simulation using 10–15 layer lumped was not still computationally practical for bulky parts. To tackle this issue, Liang et al. [86] proposed an enhanced layer lumping method (ELLM) in meso-scale modeling in which the material properties for the lumped super layers are modified to alleviate underestimation errors in the residual stress and deformation. The procedure has been shown in Fig 2.6 in which the solid black line shows the stress-strain progression once one equivalent layer n is activated. For the 2-super-layer situation, the n and $n+1$ layers are activated concurrently, where the blue dashed line depicts the stress evolution associated with the bottom layer that attains to a lower magnitude in comparison with the activation of only one equivalent layer. The same scenario can be explained for the 3-super-layer case, as the lowest layer would behave like the red dashed line, and the $n+1$ and $n+2$ layers should behave as the blue dashed and solid black lines, respectively. Despite the simultaneous activation time for multiple equivalent layers in the lumped super layer method, various stress levels would emerge in different equivalent layers. As a result, specialized material constitutive models should be employed to modify the yield stress and inherent strains for distinct layers in ELLM to reduce overestimation errors. The accuracy, scalability, and robustness of ELLM were validated on a cantilever beam and a large complicated canonical part where the 4-layer ELLM case could reduce the simulation time by 70% [86]. Promopattum and Uthaisangsuk [80] explored the importance of optimizing the number of scanning paths to account for the influence of local preheating for the thermomechanical simulation of a single layer. In addition, concerning the relationship between the part's height and compressive stress accumulation, they asserted that the stress would transfer toward the center of the part as the height of the part becomes taller.

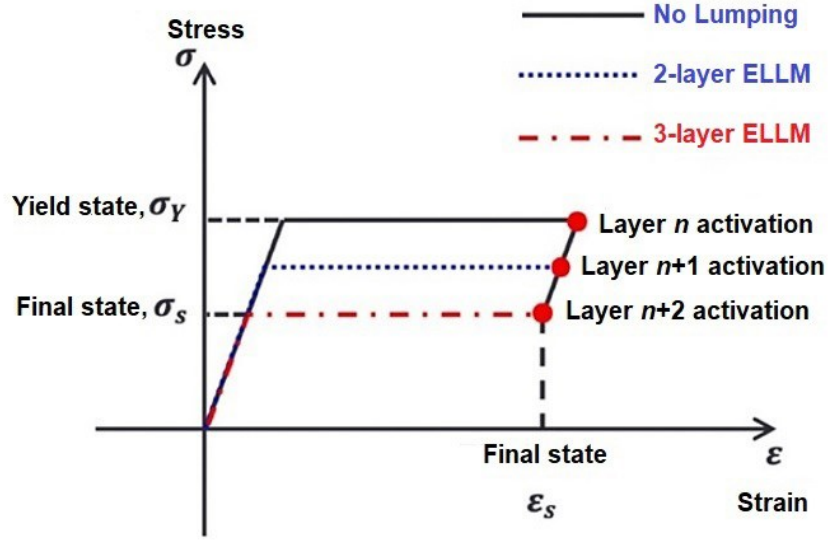


Fig 2.6 The progress of residual stress and equivalent material models as a result of 2-layer and 3-layer lumping [86]

2.3.3 Simulation of the thin-walled lattice support structure by the MISM

Due to the high computational cost of performing a non-linear thermo-mechanical analysis of lattice support structures, Liang et al. [87] achieved pioneering research in adapting the MISM to these structures using the asymptotic homogenization technique. Following the MISM in previous studies, they obtained directional inherent strains through the mesoscale modeling of thin-walled as a representative volume element (RVE) given the periodicity of the macroscopic lattice support structures as shown in Fig 2.7. An asymptotic homogenization approach [88] was then used to calculate RVE's equivalent thermal and mechanical parameters, including elastic modulus and inherent strains. After homogenizing the mechanical properties, the block made by the lattice support structure can be regarded as a solid continuum model in layer-wise simulation [87]. Not only did the postulated homogenization approach demonstrate good agreement with experimental measurements, but it also resulted in a tenfold increase in computational performance.

2.3.4 On the incorporation of scanning patterns into the MISM modeling

The laser scanning strategy is one of the crucial elements responsible for the anisotropy in the mechanical properties of parts manufactured by the LPBF process [89]. This issue confirms the longitudinal and transverse deviation in Young's modulus and yield strength of many LPBF components with respect to the laser moving direction. On the other hand, the layer-by-layer fashion rotational laser scanning method has less impact on the mechanical properties compared to the unidirectional scanning approach partially due to the high dependency of microstructures on

temperature gradients caused by the laser moving direction [89]. Concerning the impact of anisotropy on residual deformation, Liang et al. [31] investigated the effects of various laser scanning strategies included in MISM to accurately predict the residual deformation of the LPBF components. Despite the parallel line (PL) laser scanning strategy, where the directional material properties like inherent strains and elastic modulus can be implemented in a single local elemental coordinate system (LECS) toward the laser moving direction, in the rotational line (RL) laser scanning strategy, the LECS should be separately assigned to different layers according to the laser moving direction. To satisfy both accuracy and efficiency in the finite element analysis of a large model, the asymptotic homogenization method [88] was employed to extract the equivalent elastic modulus and the correct form of the modified inherent strain vector for the RL laser scanning pattern. Technically, the homogenized inherent strain vector (HISV) can be computed by assigning the directional inherent strain vector attained from small-scale modeling to a number of lumped real layers as the coefficients of thermal expansion in accordance with the laser scanning direction for each thin layer. The number of merged layers is considered a representative volume element (RVE) as the smallest repetitive volume. The height of this RVE depends on the regularity of the rotational laser scanning routes in a part. As an example, Fig 2.8 illustrates a 3-layer RVE for the 60° RL laser scanning pattern with a layer thickness of 40 μm , which shows at least 3 layers are necessary to achieve a 180° rotation of the laser scanning line relative to the initial position of the laser moving vector direction. Finally, the homogenized elastic modulus and HISV are used in a layer-by-layer fashion irrespective of the laser scanning strategies to measure the residual deformation in an efficient way [31]. The incorporation of scanning strategies into MISM has been validated by the experimental data, ensuring excellent accuracy of the proposed workflow. Besides the capability of this comprehensive method to be used in many cases involving RL laser scanning strategies, the development of this methodology with the integration of anisotropic plastic yielding law is a potential future work suggested by the authors.

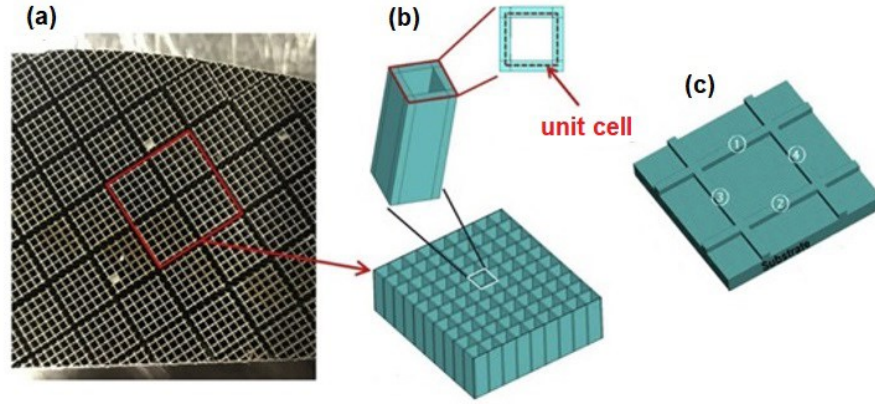


Fig 2.7 (a) The thin-walled lattice support structures in LPBF; (b) the representative unit cell (red dashed square); (c) the representative volume for small-scale modeling [87]

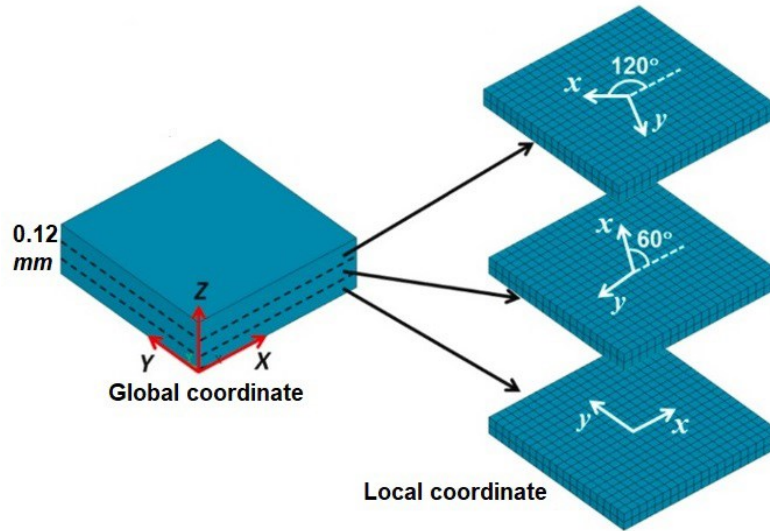


Fig 2.8 The 3-layer RVE model in the local and global coordinate systems for a 60° RL laser scanning pattern [31]

2.3.5 Improved modified inherent strain method

Although the MISM demonstrated its ability to accurately compute the residual deformation in LPBF parts, its accuracy in the residual stress prediction was still not validated. To do so, Dong et al. [90] conducted detailed investigation to evaluate the capability of the existing MISM to fairly estimate residual stress distribution without affecting the prediction of residual deformation. In the first step, a 3-layer single-walled structure was modeled to compare the residual stress accumulation between the detailed simulation results and the existing MISM. To capture a precise broad range of temperature-dependent material properties, they applied a cut-off temperature,

recommended by Lindgren [91], beyond which the material properties remain unchanged. After performing the numerical analyses, despite the good agreement in the maximum residual deformation predicted by the two processes, the obtained residual von Mises stress was overestimated by the MISM, which was much higher than the detailed simulation (close to the yield strength). Therefore, the existing MISM approach failed to measure residual stress precisely. The first attempt was to identify the potential source of the error. Due to the valid residual deformation results, they concluded that the inherent strain values measured in the mesoscale stage are trustworthy and an inaccurate relative percentage of elastic and plastic strains in total strains may give rise to an overestimation in predicted residual stress level. They reported the use of constant ambient temperature material properties in macroscale modeling may be a possible source of inaccuracy [90]. As mentioned in section 2.3.1, over the span of two phases, namely intermediate and steady state, the local and global temperature gradients induce strains, respectively. Thus, in the macroscale modeling of MISM, in order to reach an accurate proportion between the final elastic and plastic strains, both the effects of localized and global thermal gradients must be included, which implies that using just materials properties at ambient temperature cannot satisfy this condition. Based on this hypothesis, a new implementation procedure for the MIS-based simulation was proposed in which two consecutive static analyses are performed using the material properties at the intermediate and steady state temperatures, respectively, while the inherent strains are kept constant in both steps [90]. Fig 2.9 provides a detailed description of both the existing and the new MISM. As a demonstration of the new procedure's validity with respect to the detailed simulation results, the von Mises stress field for a 3-layer thin-walled model is represented in Fig 2.10 where the new MISM offers better residual stress prediction compared to the existing one. Furthermore, to assess the viability of the new MISM experimentally, the L-bracket and canonical parts were printed, and the good agreement between numerical and experimental results indicated the sound performance of the new implementation [90].

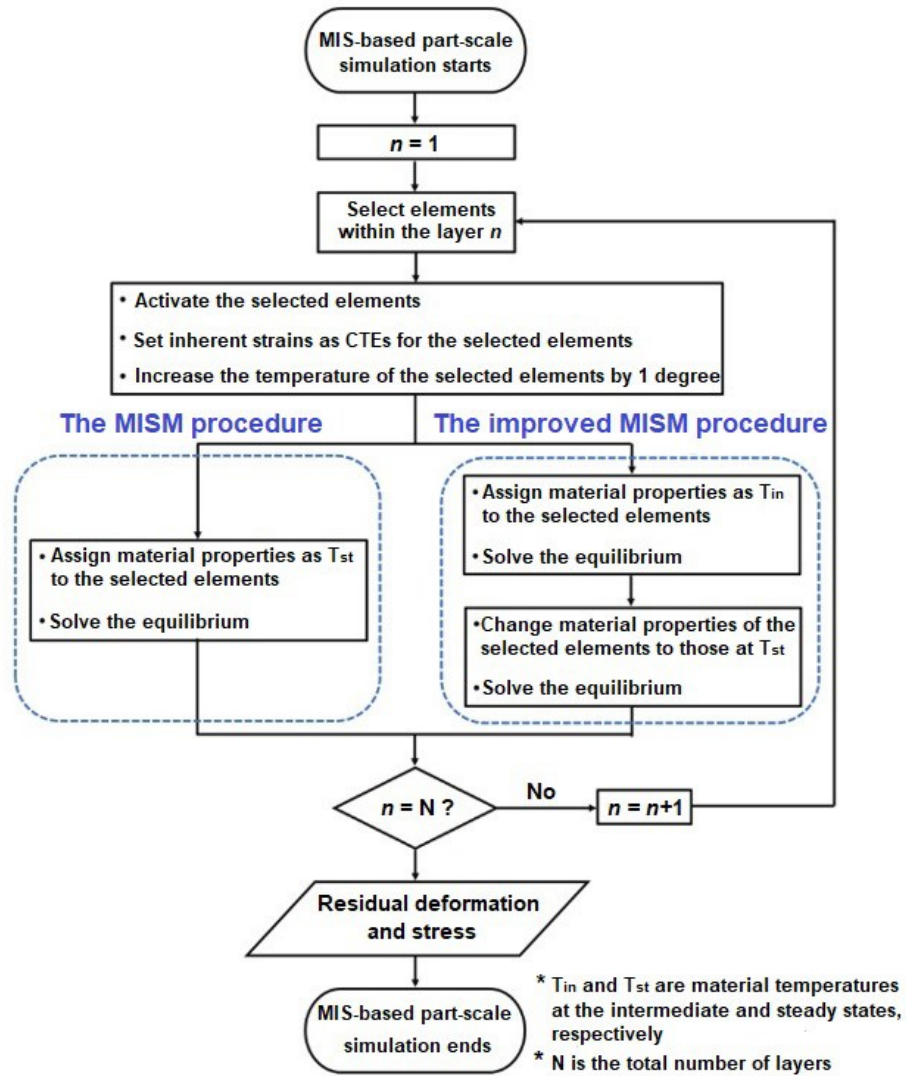


Fig 2.9 Comparison of the existing and new procedures for MIS-based part-scale simulation [90]

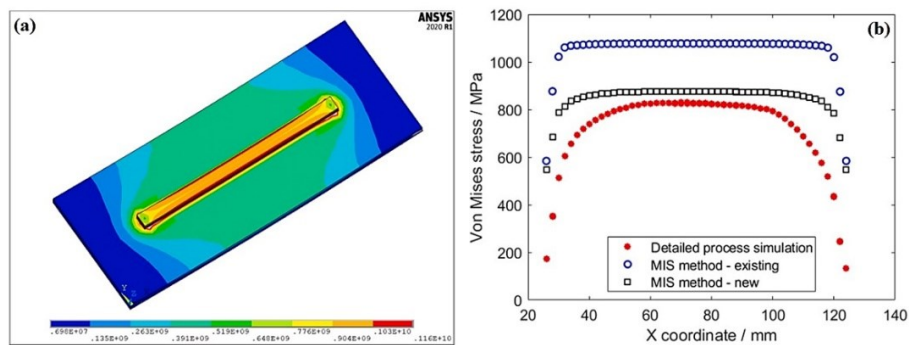


Fig 2.10 (a) Von Mises stress field; (b) comparison of the von Mises stress along the top centerline in different simulations [90]

2.3.6 Optimization based on the ISM

In the last couple of years, innovative optimization techniques based on the inherent strain method have been developed to identify the optimum design parameters with the goal of lowering the detrimental residual stresses and volume of the support structure. As the most patently examples, Cheng et al. [92] proposed a multi-objective optimization methodology to automatically define the optimal build orientation for complicated parts. In their modeling, the stress distribution in the support structure was calculated by the voxel-based fictitious domain (i.e. finite cell method) rather than the conformal mesh to avoid time-consuming mesh generation during the optimization process. It was found that not only does the suggested method mitigate the impact of residual stress in the build part, but it also secures the design manufacturability while diminishing the material consumption for the support structure. In another study, Zhang et al. [93] executed the topology optimization and inherent strain method for the support structure by considering the gravity load in the objective function to reduce the before and after-cutting deflections in printed cantilevers. Their experimental and numerical (ISM) findings revealed that the optimized supports may reduce component deflection and material consumption by more than 60% and 50%, respectively, compared to the default support structure. Examining the feasibility of the part-scale topology optimization for continuum and lattice support structure design via the inherent strain method was also carried out by other researchers [93–97]. Besides confirming previous findings on advantage of optimized support structure on mitigation of residual stress and part deformation, it was also observed that stress-induced cracking would no longer appear in the parts with optimized support structure.

As previously mentioned, according to the anisotropic nature of the local deformation caused by the moving heat source in the LPBF process, the scanning route may dramatically alter residual stress inside a component. Scanning path optimization has thus been proved to be an efficient solution in the reduction of residual stress and deformation. For instance, Chen et al. [98] proposed a novel method to perform continuous layer-by-layer scanning path optimization using the inherent strain method. A numerical strategy, namely, adaptive level set adjustment (ALSA), was employed to ameliorate the detrimental effect of disregarding a portion of the sensitivity result. Typically, the level set technique is a mathematical framework for assessing and monitoring implicit moving interfaces [99]. It was observed that the zero-level set contour continues to shrink, until it comprises a very small portion of the design domain, causing the optimization problem fails to

converge. In this situation, the ALSA technique tries to keep the zero-level set contour inside the design domain during the process optimization, achieving a good convergence for both compliance and stress minimization problems. This scalable approach demonstrated its ability to be used for parts with more complicated geometrical features, extending to integrating both topology and laser scanning path optimization simultaneously [98]. The island scanning pattern optimization method was another study conducted by Chen et al. [100] to reduce part deformation. Considering the scanning orientation-dependent inherent strain vector associated with each island in a given geometry as a design variable, finite element analysis was used to determine the optimal scanning direction for each island through an iterative optimization algorithm. The feasibility and effectiveness of the suggested method were experimentally validated on a block structure and a connecting rod. A considerable reduction in residual deformation of the two parts was achieved by over 50 % compared with the initial scanning pattern.

The principle for hatch pattern optimization was explored by Li et al. [101] via developing an innovative neural network-based model, capable of predicting inherent strains for any given hatch pattern used in the part build. They trained a feedforward propagation neural network model with inherent strain values obtained from an initial hatch pattern and validated with the inherent strain data attained from subsequent hatch pattern using the microscale detailed simulation. The neural network examines the correlation between the hatch angles of various layers to determine the total inherent strain. Fig 2.11 represents the overall methodology of the suggested approach step by step. It was shown that trained neural network could estimate the inherent strain of any randomly hatch pattern with less than 8% inaccuracy.

2.4 Practical implications of the research

This section highlights some of the practical implications of this research derived from two components reviewed previously in this paper. In the optimization-based problems, the numerical method may require hundreds of iterations to converge, and each iteration demands a part-scale residual stress calculation. Using a high-fidelity ISM-based numerical model in which the LPBF process is replicated based on the actual process parameters can be the most accurate and efficient way to predict the residual stress and distortion. The salient feature of the inherent strain approach is that it replaces the computationally costly detailed thermo-mechanical simulation with a pure mechanical analysis. This enables physics-based iterative optimization to systematically remove

residual stress-induced build failure [92]. Moreover, when lattice support structures are employed in build of the parts with overhanging structure, the detailed simulation of the LPBF process becomes more complicated due to the difficulty in mesh generation and the implementation of the exact laser scanning strategy and process parameters. Using the ISM can facilitate to efficiently predict the residual deformation of those AM components with open-cell lattice structure in terms of topological features and physical printing manners. Therefore, due to the wide range of industrial applications for the parts fabricated by the LPBF, the implementation of high-fidelity and efficient numerical methods such as the ISM, not only the computational cost is significantly reduced, but in terms of sustainability, it may establish an industry that is smarter, and more efficient (less material waste and faster supply chains).

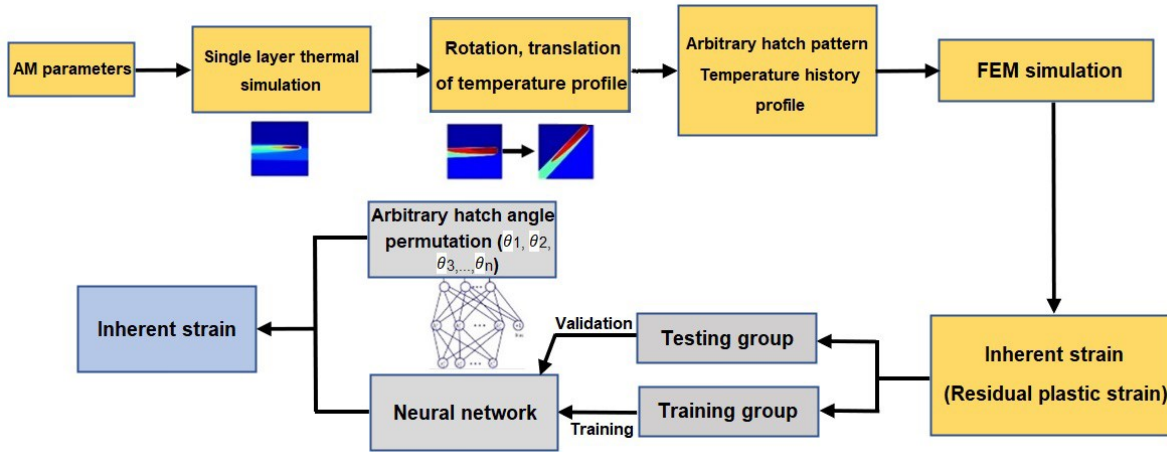


Fig 2.11 Flowchart of the proposed neural network-based method to predict inherent strain [101]

2.5 Conclusions and future directions

In this paper, a detailed review is performed on the development of the inherent strain method as an efficient technique compared to the conventional thermo-mechanical simulation in LPBF additive manufacturing process. A brief discussion was first presented on the coupled thermo-mechanical simulations, including their energy, temperature-displacement, and governing mechanical formulations. Due to the inaccurate residual stress and deformation predictions resulting from the original inherent strain method, the proposed modified version demonstrated its ability to provide a more precise analysis of inherent strains considering the contribution of residual strain in the intermediate and final steady states of the depositions. Moreover, the application of the MISM to the thin-walled lattice support structure by using the asymptotic homogenization method was reviewed demonstrating its capability to dramatically enhance the

computational performance. It was shown that the improved MISM can predict the residual stress in excellent agreement with experimental results by taking into account the effect of both local and global thermal gradients on the temperature-dependent material properties.

Thus far, much research has been conducted using the inherent strain method to evaluate the influence of some contributing factors, such as layer lumping effect, scanning strategy, and process optimization on the formation of residual stress and deformation. However, there are still some important parameters like strain and rate of hardening in the plastic yielding law or the influence of phase transformation in the microstructure evolution [102] that can be a potential source of error since they were overlooked in the majority of the recent inherent strain-based investigations. Therefore, it is expected that future research attempts will be directed toward determining the effect of these characteristics on the prediction made by the MIS approach. On the other hand, incorporating machine learning methods such as neural networks to connect a large number of process parameters to the associated inherent strains is a captivating outlook by which a large database can be used to train the neural networks with the aim of building a relationship between undeformed and deformed geometry, compensating for the distortion in the metal parts [103]. Moreover, formal design optimization formulation to identify optimal process and geometrical parameters in the LBPF to minimize the part distortion due to induced residual stresses has not been investigated. Combination of high-fidelity validated finite element model and deep learning artificial intelligence algorithm as a growing trend may provide unique opportunity to develop computationally efficient reduced order models to be practically used in optimization formulation.

Chapter 3 Development of an efficient multi-scale model to predict residual stresses and distortions in the laser powder bed fusion process for Inconel-718

Abstract: In the Laser Powder Bed Fusion (LPBF) process, fast solidification of molten powders and significant temperature gradients generate substantial residual stresses in the build part. The induced residual stresses can result in excessive deformation and potential crack initiation and propagation. Development of a predictive reliable model is thus of paramount importance to predict the induced residual stresses in LPBF process without cost and complexities associated with experimental tests. High fidelity thermo-mechanical models to predict the residual stresses and distortion in the macroscale are generally impractical owing to their high level of computational time. Recently, the modified inherent strain methodology has proven to be a viable alternative for predicting residual stresses and distortions efficiently. In this study, a multi-scale finite element-based model of the LPBF process for Inconel-718 is developed utilizing modified inherent strain method to estimate the accumulated stress in the process. The stress formation and inherent strain values were evaluated in a microscale deposition considering the effect of LPBF process parameters using Abaqus/standard. The material constitutive models, including kinematic hardening, elastic-perfectly plastic, isotropic hardening, and Johnson-Cook models, and their effect on the evolution of plastic strain were investigated. The precision of the prediction was examined based on the quantity of equivalent layers, employing the agglomeration approach in part-scale analysis, and subsequently confirmed experimentally through the fabrication of a printed cantilever beam. The proposed framework showed that the kinematic hardening model performed better than other material models, with an error of less than 6% when compared to experimental measurements. Moreover, the study highlights the significance of selecting the most appropriate material model for future studies involving the integration of advanced artificial neural networks and process parameter optimization to achieve precise and computationally efficient predictions.

3.1 Introduction

In the field of additive manufacturing (AM), laser powder bed fusion (LPBF) has proven to be the most popular method for fabricating metal parts. In the LPBF process, a thin layer of metal powder is melted and solidified by a fast and intense moving heat source following a predefined scanning path, thereby creating a 3D component layer by layer. Due to the highly concentrated laser power and large local energy density [1], a considerable temperature gradient, phase change transformation, and rapid heating and cooling cycles occur that induce a considerable amount of residual stresses and subsequent distortions in the fabricated components [2,30]. The need to assess residual stresses and distortions in design and optimization of parts has prompted the exploration of various techniques for evaluating the effect of these factors in parts produced through the LPBF process. While the complex physics of the LPBF process necessitates experimental investigation, the costly and time-intensive nature of these experiments has led researchers to develop predictive thermo-mechanical models to efficiently determine how the temperature gradients and induced thermal stresses and distortions evolve over time [104]. Generally, conceptual frameworks of LPBF process simulation are classified as microscale, and macroscale (part-scale) models in terms of their fidelity [3,4]. The microscale model may investigate fluid dynamics of molten pools and microstructure development at a scale of micron [5–7]. On the other hand, many complicated mechanisms associated with the melt pool and consolidation are disregarded by the macroscale model to have a computationally efficient analysis. For instance, Goldak's double ellipsoidal and Gaussian models are employed to replicate the moving heat source, and the temperature, stress, and strain profiles are calculated by conducting a coupled thermo-mechanical simulation [3,90].

Although a detailed thermo-mechanical analysis [8–10] allows for a multi-layer investigation of residual stress and distortion through the use of thermal source models [11–13], this approach is quite inefficient and computationally very expensive for part-scale prediction [14]. Therefore, to overcome the huge computational burden, some simulation methodologies were developed like the classical inherent strain (IS) method, plastic strain method, and agglomeration (layer lumping) approach [16,20,21,105,106]. The classical IS method was introduced for the first time to estimate the deformation in the metal welding process [104]. In this method, the stress and strain fields in the distorted welded structures are simulated by applying inherent strains to undeformed models with completely elastic material behavior. The IS values can be obtained using either empirical strain measurements on weld samples or numerical simulations of the welding process. Following

complete cooling to room temperature, the residual plastic strains are calculated to extract the IS in welded structures. Total distortion is then predicted by applying the resulting plastic strain tensor to a real component and conducting a linear elastic analysis. However, it was shown that the classical IS method cannot provide accurate prediction for the distortions in the complex additively manufactured parts [23,27,30].

Furthermore, the applied plastic strain approach, inspired by the IS method, was developed for predicting welding distortion [17,18]. However, it was observed that the precision of this approach is not enough when used to large additive manufacturing structures. This limitation arises from the agglomeration approach, where numerous computational layers are combined to create an equivalent layer, resulting in a significant reduction in both mesh size and overall time-step [12]. Nevertheless, due to high computational costs, the utility of this approach was also restricted [80]. In another study, Setien et al. [26] proposed a technique to determine the inherent strains in Ti-6Al-4V based on the classical laminate theory (CLT) in composite laminates. The unique IS values that correspond to each layer were found by repeatedly optimizing the difference between predicted residual distortions and experimental findings of twin cantilever beams. Despite its precision, the necessity for numerical optimization and the manufacture of a large number of samples limit the industrial use of this expensive technique [104]. Recently, Liang et al. [23] developed a modified inherent strain (MIS) method to account for the fast-moving heat source and multi-layer build model of additive manufacturing in comparison to the welding process in order to achieve more precise IS values. The modified version includes the definition of material behavior and contains the IS values in both the ambient temperature and elevated temperature above melting point. The MIS method analysis is carried out in a layer-by-layer part-scale model. Good agreement between the numerical and experimental results revealed the robust performance of the MIS especially for predicting the distortions in the large and geometrically complex parts [27,30,87]. Later, Dong et al. [90] conducted a thorough investigation to enhance the accuracy of MIS method in estimating residual stress while maintaining the accuracy of distortion predictions. Thus far, several studies have been performed on the improvement of the MIS method accuracy and efficiency [31,86,92,93,95,96,100]. In all studies, the material constitutive model was assumed to be elastic-perfectly plastic, and the investigation was conducted based on the influence of AM processing parameters. However, characterizing material properties is as important as process parameters for determining accumulated stress and distortion. For instance, Promoppatum and

Rollett [107] investigated that neglecting rate-dependent hardening reduces the calculated stress in the LPBF of Ti-6Al-4V by 20%.

To date, there has been a lack of comprehensive exploration into incorporating strain and the rate of hardening into the plastic yielding law for IS-based LPBF simulation. Addressing this aspect could potentially reduce the computational time in predicting residual stress and distortion using the IS method. Therefore, the main objective of this research study is to extract IS values using the MIS method and assess the impact of hardening on the prediction of residual stress and distortion in Inconel-718. To accomplish this, elastic-perfectly plastic (EPP), isotropic (IsoH) and kinematic hardening (KinH), and Johnson-Cook (JC) models are considered as the material constitutive laws. The JC model is utilized since it can accurately represent how a material responds to strain and strain rate at high temperatures.

The remainder of the paper is arranged as follows: In Section 3.2 the MIS method is reviewed. In Section 3.3 the thermal and mechanical governing equations are presented, followed by discussing the overall multi-scale numerical strategy in this research and the way of its implementation in Abaqus. Then in Section 3.4, results and discussion are provided to evaluate the influence of material models with respect to the number of equivalent layers. The results are compared with experimental measurement of a cantilever beam. Finally, conclusions and future remarks are presented in Section 3.5.

3.2 Modified inherent strain (MIS) method

The concept of MIS method is inspired by the classical inherent strain theory in welding mechanics which assumes the total strain in the welded part can be computed as follows:

$$\varepsilon_{total} = \varepsilon_{elastic} + \varepsilon_{plastic} + \varepsilon_{thermal} + \varepsilon_{creep} + \varepsilon_{phase\ transformation} \quad (\text{Eq 3.1})$$

Based on the theory of classical IS method, the thermal strain disappears at the final cooled stage and the rest of the inelastic strains except the plastic strain can be disregarded due to their infinitesimal values. Therefore, the plastic strain is attributed to the inherent strain value since it always remains in the part while the elastic strain is completely released. The classical theory defines inherent strain as below:

$$\varepsilon_{classical}^{inherent} = \varepsilon_{total} - \varepsilon_{elastic} = \varepsilon_{plastic} \quad (\text{Eq 3.2})$$

However, the classical theory falls short in providing precise predictions of residual stress and distortion for LPBF. This limitation arises from the construction of a multi-layer model with a rapidly moving heat source, leading to the influence of layer-by-layer contraction of the upper layers on the elastic deformation and stress development in lower layers. To address this limitation, the MIS method was introduced to minimize inaccuracies. This is achieved by accounting for the contribution of large compressive plastic and elastic strains ($\epsilon_{mechanical}^{int}$) at the highest temperature once the heat source passes a specific point of interest at the first layer. Additionally, the method considers the inter-layer effect and thermal contraction when the built part cools down to ambient temperature ($\epsilon_{elastic}^{ss}$). These two factors are introduced as the intermediate and steady states, respectively. The modified inherent strain value is computed as the difference between the overall mechanical strain at the intermediate stage (plastic and elastic strains at a specific point of interest in the bottom layer after the deposition of the subsequent layers are completed with the condition of remelting of the first layer) and the steady-state elastic strain (elastic strain at the specific point of interest in the bottom layer as the part cools down to ambient temperature) [30], as follows:

$$\epsilon_{modified}^{inherent} = \epsilon_{mechanical}^{int} - \epsilon_{elastic}^{ss} \quad (\text{Eq 3.3})$$

where *int* and *ss* stand for the periods of time that correspond to the intermediate and steady states, respectively. According to Eq 3.3, the difference between elastic strain at intermediate and steady states is regarded as the amount of thermal strain transformed into deformation at the final cooled stage compared to the classical IS method. Fig 3.1 illustrates the development of compressive elastic and plastic stress and strain during the first stages of powder sintering, which eventually change into tensile stress and strain due to a fast-cooling rate. At high temperatures, the non-uniform thermal expansion caused by a strong temperature gradient in front of the melt pool region is constrained by nearby solidified metals, leading to the generation of initially compressive stress and strain at the intermediate state. After the heat source passes, the desired point cools down rapidly, and the compressive thermal stress and strain eventually become tensile as a result of thermal contraction in the area behind the heat source. In fact, the deformation of the material at the specific point of interest in the bottom layer progressively changes. Additionally, within a multi-layer deposition, it was noted that the plastic strain of the bottom layer remains relatively unaffected by successive layer depositions after cooling, unlike the more pronounced alternations

observed in elastic strain. [30,90]. Therefore, the modified inherent strain equation considers the relaxation of elastic strain at the final cooled condition (steady state).

3.3 Numerical modelling

3.3.1 Thermal analysis: thermal properties, governing equations, boundary conditions, and heat source model

The governing equation describing the LPBF process can be represented by heat conduction Fourier equation and application of appropriate boundary conditions as below [108]:

$$\rho c_p \frac{dT}{dt} = \frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial T}{\partial z} \right) + Q(x, y, z, t) \quad (\text{Eq 3.4})$$

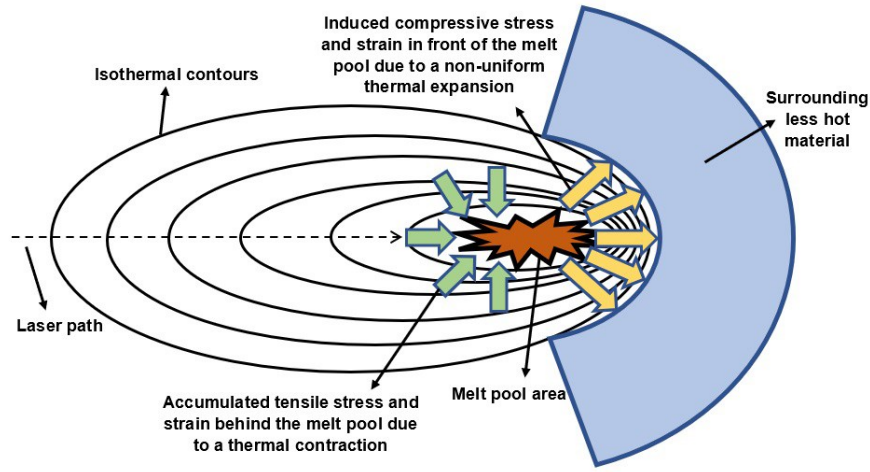


Fig 3.1 Formation mechanism of the compressive/tensile stress and strain due to thermal expansion and contraction in the melt pool area

Where ρ is the material density, c_p is the temperature-dependent specific heat, k_x, k_y, k_z are the anisotropic temperature-dependent thermal conductivity of x, y, z directions, T is the temperature and Q is the internal heat generation per unit volume. In terms of boundary conditions, the convection heat transfer with the ambient environment is applied to the deposition layer and surrounding powder layer based on Newton's law:

$$q_c = -h_c(T_{ext} - T_{\infty}) \quad (\text{Eq 3.5})$$

where q_c , h_c , T_{ext} and T_{∞} are heat dissipation, heat transfer coefficient, geometry temperature, and ambient temperature.

Furthermore, heat loss radiation from the geometry domain is introduced as follows:

$$q_r = -\sigma\varepsilon(T_{ext}^4 - T_\infty^4) \quad (\text{Eq 3.6})$$

where q_r , σ and ε are heat dissipation, the Stefan-Boltzmann coefficient, and the emissivity coefficient. In general, the following equation can be used to represent all boundary conditions [109]:

$$k \frac{\partial T}{\partial n} + h_c(T_{ext} - T_\infty) + \sigma\varepsilon(T_{ext}^4 - T_\infty^4) - I = 0 \quad (\text{Eq 3.7})$$

in which I is the external heat source. The bulk thermal characteristics of Inconel-718 as a function of temperature can be found in [59,80]. To account for the porosity effect in metallic powder, different models of thermal conductivity have been offered [110–112]. Since the thermal conductivity is also influenced by the surrounding gas contained inside the voids, an empirical equation was formulated for the effective conductivity of a packed bed considering the conduction, convection, and radiation effects within a powder bed as [113]:

$$k_{eff} = \frac{\mu k_b}{1 + \gamma k_b/k_g} \quad (\text{Eq 3.8})$$

where k_b is the temperature-dependent thermal conductivity of the bulk material, k_g is the temperature-dependent thermal conductivity of surrounding gaseous environment, $\mu = \rho/\rho_b$ (where ρ_b is the density of the bulk material) and the empirical coefficient $\gamma = 0.02 \times 10^{2(0.7-\mu)}$. The solidus and liquidus temperatures are defined to account for the powder-liquid-solid transition. The powder material begins to melt at the solidus temperature and liquefies completely at the liquidus temperature. The apparent heat capacity approach [114] is used to account for the transition from the solid to liquid state:

$$c_p = \begin{cases} c_{p,sensible} & T < T_S \text{ or } T > T_L \\ c_{p,sensible} + \left(\frac{L}{T_L - T_S} \right) & T_S < T < T_L \end{cases} \quad (\text{Eq 3.9})$$

where L, T_S, T_L are the latent heat, solidus, and liquidus temperatures, respectively. In thermal modelling, the heat source model is essential to accurately replicate the heat input. While some research studies simply represent the heat source as a temperature load [37,115], the moving

Gaussian heat source is widely utilized consisting of scanning speed and time effects. For the volume-related heat source, Goldak's semi-ellipsoidal shape was applied for modeling the melt pool dimensions and temperature distributions (Fig 3.2). The Goldak heat source is described as follows [11,108]:

$$I(x, y, z) = \frac{6\alpha\sqrt{3}P}{\pi\sqrt{\pi}abc} \exp \left[-3 \left(\frac{x^2}{a^2} + \frac{y^2}{c^2} + \frac{z^2}{b^2} \right) \right] \quad (\text{Eq 3.10})$$

where $I(x, y, z)$, α , P , a , b , c are heat intensity distribution, laser absorptivity, laser power, and dimensions of the heat source profile, respectively. By considering the boundary conditions, the external heat source $I(x, y, z)$ and losses are fed from Eq 3.7 into Eq 3.4 to calculate the internal generated heat $Q(x, y, z, t)$.

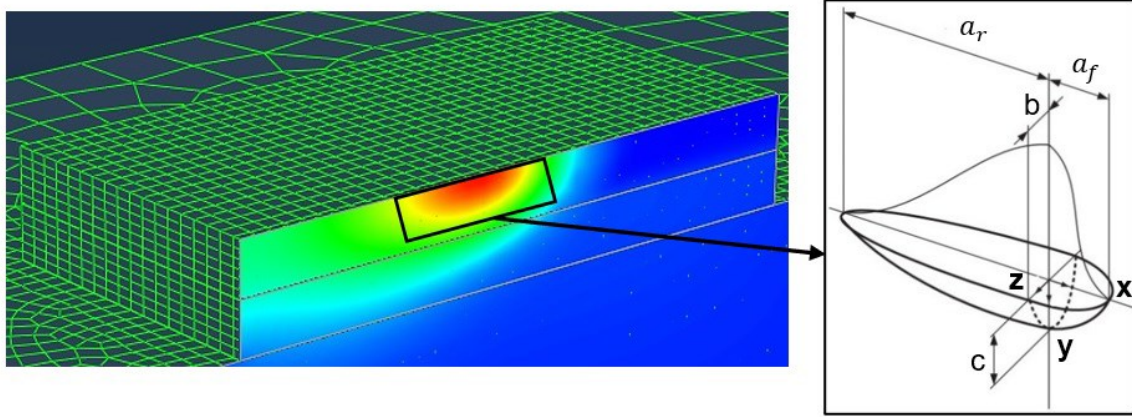


Fig 3.2 Volumetric Goldak heat source shape

3.3.2 Mechanical analysis: material properties and material constitutive models

The mechanical response for the microscale model is obtained using the estimated temperature field evaluated from the pure heat transfer analysis. A cut-off temperature was established in order to precisely capture a wide range of temperature-dependent material properties, ranging from room temperature all the way up to the melting point and even higher temperatures. This was accomplished by determining a temperature beyond which the material properties do not change [91]. To account for a very accurate simulation, $T_{cut-off} \geq T_m$ was considered for the young modulus and thermal expansion coefficient. Due to the significant decrease of the young modulus at the melting point, it is linearly reduced from the value at about $0.7 T_m$ to a very small value at the cut-off temperature. In addition, since above the liquidus temperature, there is only

solidification shrinkage and the thermal strains would not accumulate, the thermal expansion coefficient was defined as zero at the melting point. Fig 3.3 shows a schematic representation of the $T_{cut-off}$ for some physical constants of Inconel-718.

The constitutive incremental stress-strain relation can be written as below:

$$d\sigma_{ij} = D_{ijkl}(d\varepsilon_{kl}^t - d\varepsilon_{kl}^p - d\varepsilon_{kl}^{th}) \quad (\text{Eq 3.11})$$

where σ is the Cauchy stress tensor, D is the fourth order stiffness tensor, and the incremental plastic strain $d\varepsilon^p$ is calculated using the corresponding flow rule equation as follows:

$$d\varepsilon_{ij}^p = d\lambda \frac{\partial f}{\partial \sigma_{ij}} \quad (\text{Eq 3.12})$$

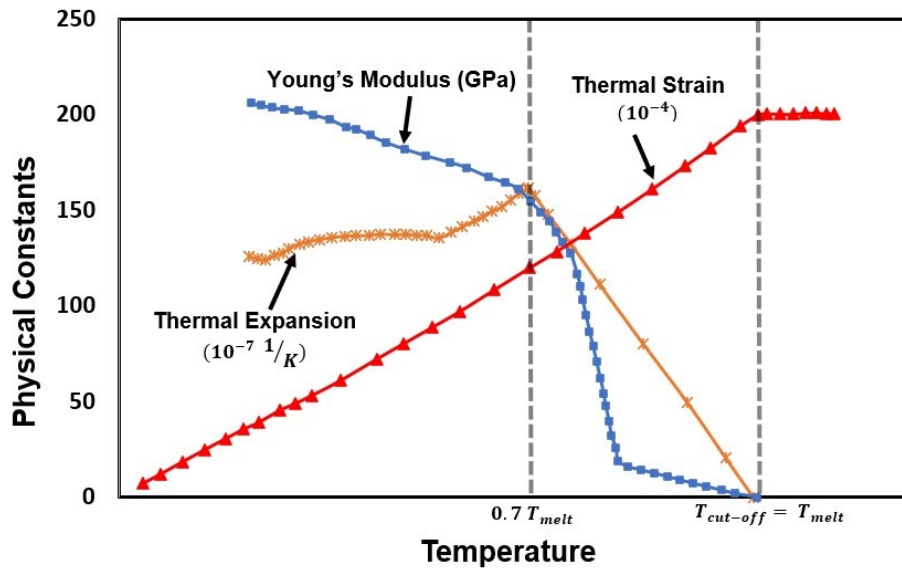


Fig 3.3 Schematic illustration of the cut-off temperature for material properties of Inconel-718

In Eq 3.12, $d\lambda$ is a positive scalar factor of proportionality that is identified to be nonzero when plastic deformations are existent [116]. $d\varepsilon_{ij}^t$ is determined by the total of incremental elastic, plastic, and thermal strains. The thermal strain is defined as:

$$\varepsilon_{ij}^{th} = \int_{T_{ref}}^T \alpha_{ij}(T) \delta_{ij} dT \quad (\text{Eq 3.13})$$

where α_{ij} is a temperature-dependent thermal expansion coefficient tensor and δ_{ij} is the Kronecker delta. Many practical applications rely on the premise that a material exhibits minimal strain hardening. Consequently, it is assumed that plastic deformation occurs under a constant flow stress, known as perfectly plastic behavior. This assumption can considerably simplify the analysis of complex geometric structures. In this case, the J_2 von-Mises yield criterion, alongside the flow rule, is applied in the form below to determine the plastic strain [116]:

$$f(\sigma_{ij}) = \frac{1}{2} s_{ij} s_{ij} - S_y^2 = 0 \quad (\text{Eq 3.14})$$

where s_{ij} is the deviatoric stress tensor and S_y is the yield strength that is calibrated through the uniaxial tensile test. As long as the stress point remains above the yield surface, plastic deformation proceeds. The loading and unloading conditions are controlled by the state of stress that must either stay on the yield surface and maintain the plastic flow or drop below the yield point and eliminate the plastic deformation. On the other hand, engineering materials often display strain-hardening characteristics. In this situation, an increase in the stress magnitude over the initial yield surface into the work hardening zone causes plastic and elastic deformations. During each level of plastic deformation, a new yield surface is generated. This kind of behavior depends on the loading path relative to the initial yield surface. The constitutive equations associated with the strain-hardening effect also follow the flow rule. According to the IsoH von Mises model given by Eq 3.15, the size of the yield surface is controlled by the value φ , which relies on the plastic strain history. This hardening rule implies that when plastic flow occurs, the initial yield surface expands continuously with no deformation or translation [116].

$$f(\sigma_{ij}, \varphi) = \frac{3}{2} s_{ij} s_{ij} - \varphi^2(\bar{\epsilon}_p) = 0 \quad (\text{Eq 3.15})$$

The hardening parameter $\varphi(\bar{\epsilon}_p)$ is linked with the effective plastic strain $\bar{\epsilon}_p$ experimentally through the uniaxial stress-strain curve. Moreover, the KinH rule offers a straightforward solution for the Bauschinger effect which is ideal for a full reversal of loading circumstances. In this case, the loading surface transfers as a rigid body in the stress space, and the size, shape, and orientation of the initial yield surface remain unchanged throughout the plastic deformation. The general form of the loading surface equation is as follows [116]:

$$f(\sigma_{ij}, \varepsilon_{ij}^p) = \frac{3}{2}(s_{ij} - \beta_{ij})(s_{ij} - \beta_{ij}) - S_y^2 = 0 \quad (\text{Eq 3.16})$$

where β_{ij} is the back-stress tensor, which varies with plastic deformation. Furthermore, a combination of IsoH and KinH would result in a more general mixed hardening rule, whereby the loading surface undergoes a translation specified by β_{ij} and a uniform expansion calculated by φ^2 , but keeps its initial shape. With the mixed hardening rule, different degrees of the Bauschinger effect can be simulated by simply adjusting the two hardening parameters β_{ij} and φ^2 . When a J_2 -material is subjected to a mixed hardening rule, the general form of the subsequent loading surface is described as below [116]:

$$f(\sigma_{ij}, \varepsilon_{ij}^p, \varphi) = \frac{1}{2}(s_{ij} - \beta_{ij})(s_{ij} - \beta_{ij}) - \varphi^2(\bar{\varepsilon}_p) = 0 \quad (\text{Eq 3.17})$$

The subsequent yield surface for different types of hardening rules is illustrated in Fig 3.4.

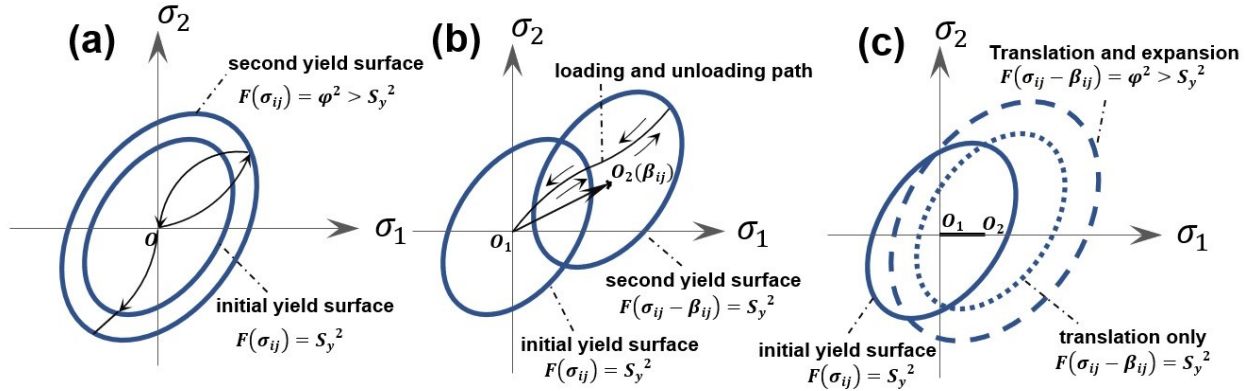


Fig 3.4 Subsequent yield surface for a) IsoH; b) KinH; c) mix hardening material

In this study, the JC plasticity model [83] is also employed to investigate the effect of strain hardening, rate dependent hardening, and temperature on the predicted mechanical responses. The JC model is a particular type of Mises IsoH that can determine the static yield strength at nonzero strain rate in the yield criterion for relatively fast processes as below:

$$S_y(\bar{\varepsilon}_p, \dot{\varepsilon}_p, T) = [A + B(\bar{\varepsilon}_p)^n] \left[1 + C \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{ref}} \right] \left[1 - \left(\frac{T - T_{ref}}{T_m - T_{ref}} \right)^m \right] \quad (\text{Eq 3.18})$$

in which $\dot{\varepsilon}_p$ is the equivalent plastic strain rate, T is the temperature of material, T_{ref} is the reference temperature, and T_m is the material melting point. The five model parameters of the JC

model including the A , B , C , n and m are material constants obtained from a quasi-static test at room temperature. The constants for the JC model of Inconel-718 are shown in Table 3.1.

Table 3.1 JC material parameters for Inconel-718 [117]					
A (MPa)	B (MPa)	C	n	m	$\dot{\epsilon}_{ref}$
1377	1243.5	0.0045	0.6767	1.29	1

3.3.3 Overview of the entire numerical approach

Having introduced the thermo-mechanical equations of the LPBF process, this section discusses the finite element simulation techniques used in Abaqus/Standard to mimic the physical phenomena occurring in the LPBF process. The following is an overview of the key methodologies that are used in the implementation of Abaqus user subroutines as well as the elements activation strategy in the microscale and part-scale analyses. The overview of the entire multi-scale modeling scheme in the MIS method is illustrated in Fig 3.19 in Appendix 3A.

3.3.3.1 Microscale single track simulation

In order to capture melt pool geometries in a microscale model, a substrate domain of $0.5 \times 0.5 \times 0.25$ mm with the powder layer thickness of $60 \mu\text{m}$ on top was considered. A hexahedral mesh size of $10 \times 10 \times 5 \mu\text{m}$ was generated, with finer mesh size implemented in regions close to the laser-material interaction zone, as depicted in Fig 3.5. To experimentally measure the melt pool, the RENISHAW AM 400 LPBF system was employed. An Inconel-718 substrate was 3D printed on a stainless-steel base plate. Subsequently, for the set of process parameters, four single tracks were generated on the substrate. All individual tracks underwent sectioning using wire-EDM, followed by polishing and etching to measure the geometrical features of melt pools. Fig 3.5(b) illustrates the fabricated base plate and four single tracks. The geometrical features of melt pools were measured using an optical microscope. Each individual track was measured at multiple locations to determine the average width and height dimensions of the melt pool. Due to the high computational time associated with the detailed thermo-mechanical simulation, an approximation must be considered for single-track modeling. According to the literature [30], it was shown the heat source model affects far-field temperatures just as much as it does on near-field temperatures. This means that model calibration using the microscale can capture the melt pool geometries similar to the part-scale when enough distance is considered concerning the expected melt pool dimensions. In addition, the bulk material below the powder layer must have a sufficient thickness to allow for

accurate calibration of the melt pool height. Therefore, the discrepancy in the dimensions between the simulation and the actual experiment does not affect the final measurement.

In this study, the validation of the numerical model involves using laser power, scanning speed and layer thickness values as indicated in Table 3.2.

Table 3.2 Process parameters used in the melt pool calibration

Process parameters	Values
Laser power (W)	200
Scanning speed (mm/s)	600
Layer thickness (μm)	60

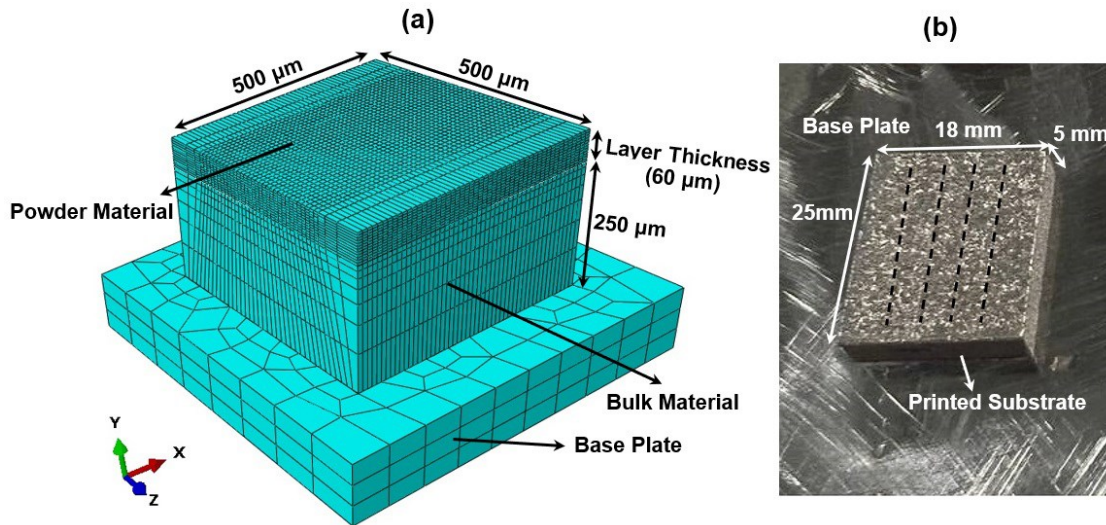


Fig 3.5 (a) Simulated single-track model geometry and mesh, (b) Produced single-track on printed substrate

The properties of Inconel-718 material for bulk and powder states were assigned to their respective domains. To account for the phase transition from powder to solid phase, the USDFLD user subroutine was used to track the material field variable. To achieve this, the thermal conductivity was first described as the powder type, transitioning to the bulk properties at the melting point. In the process of calibrating the numerical model, modifications were applied to the Goldak heat source parameters, including a , b , c , and absorption coefficient (α). These adjustments were made with the aim of reducing the difference between the dimensions of the melt pool observed in experiments and those predicted by simulation. The a , b , and c dimensions were set to initial

values. The absorption efficiency was modified between 0.4-0.6 [59,118] for acquiring more accurate melt pool shapes. Then, the parameters of the absorption coefficient and the heat source dimensions were adjusted such that the variance between the numerical and experimental data of melt pool depth and width was within an acceptable range. Due to the complexity of the LPBF process, which incorporates multiple modeling assumptions, the literature indicates that a $\pm 30\%$ difference between experimental and numerical results is allowable [119]. Fig 3.6 demonstrates that the melt pool geometries obtained from experimental measurements exhibit good agreement with the simulation results. The melt pool width and depth variations between model and experiments are below 10%. In addition, a conical-Gaussian heat source was used to examine the impact of heat source type on the dimensions and temperature gradient of the melt pool and almost identical width, depth, and temperature distributions were observed for the set of process parameters, aligning with the previous research findings [108].

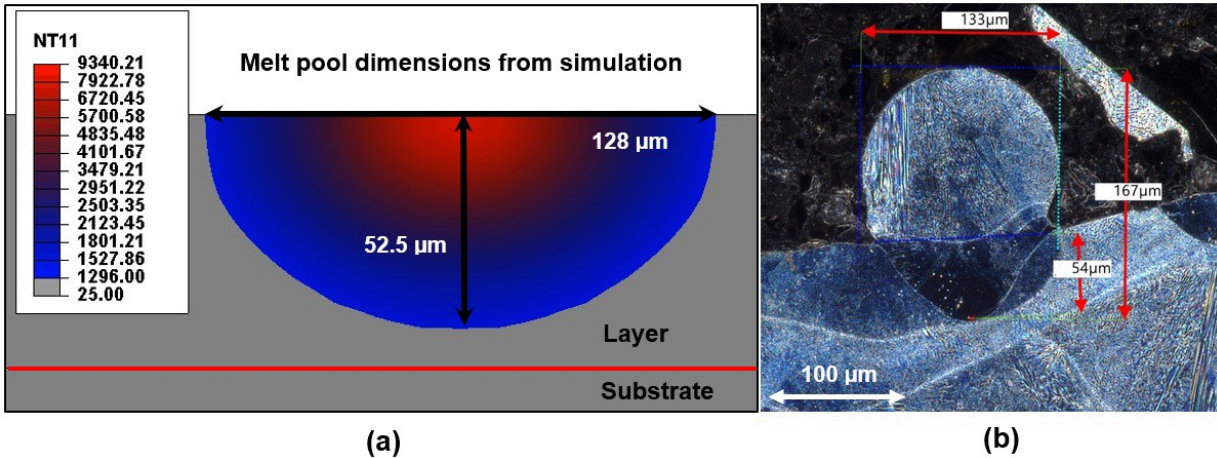


Fig 3.6 Results from (a) simulation, and (b) experiment on melt pool geometry

3.3.3.2 Microscale modeling scheme

Thermal and mechanical analyses were sequentially performed in the simulation of a three-layer deposition on the microscale. The computational domain and scanning strategy are shown in Fig 3.7. A 90° rotational scanning pattern was considered. On the basis of the physical process parameter, the values of the melt pool dimension were determined and listed in Table 3.3. The element type utilized for the heat transfer simulation was DC3D8 as an 8-node linear heat transfer brick 3D element. The elements in the powder layers have a uniform size of the $10 \times 10 \times 5 \mu\text{m}$. It was chosen as the finest possible size to achieve a good compromise between computational time and accuracy. According to the thermal boundary conditions, the top surface of the substrate and

deposition were subjected to forced convection and radiation. The convection coefficient and surface emissivity were set to 55, 0.3, respectively [30]. The initial temperature of the powder layers and building platform were set as 25 °C and 80 °C, respectively. In the thermal analysis, the elements were activated layer-by-layer and the Goldak heat flux was applied by DFLUX user subroutine to replicate the laser beam's temporal and spatial motion. The transition from the powder to solid phase was characterized by the procedures conducted during the melt-pool calibration. The temperature fields surrounding a melt pool, the thermal history of point of interest at the 1st layer, and the field variable used to determine a phase transition are displayed in Fig 3.8. As can be seen, when the laser beam travels, the elements in the region of the melt pool attain the melting temperature and are designated by the field variable of 1. Therefore, the thermal conductivity changes to bulk material. Fig 3.8(b) illustrates three separate temperature peaks corresponding to a point of interest in the lower layer, each followed by a very rapid cooling process that happens within a few seconds. The first temperature peak is a result of the first deposition, whereas the second two peaks are a result of depositing further layers. Therefore, almost the same temperature history is observed for any point in the bottom layer (no matter where the point is located). The model for the mechanical analysis was meshed using C3D8R element which is the 8-node brick element type with reduced integration point. The temperature field obtained from transient thermal analysis is subsequently applied as a thermal load. All the elements are deactivated at the beginning, and they are reactivated during the process by definition of a volume of elements. The size of the volume is calculated based on the thickness of deposition, the laser velocity in the deposition direction, and the current time increment such that the elements within the volume have a temperature greater than 5% of the melting temperature. This condition ensures that all the elements in the vicinity of the melt pool will be reactivated. After the deposition of each layer is completed, a 10-second cooling step is incorporated into the analysis to imitate the process of powder material deposition for the subsequent layer. To address convergence issue in Abaqus above melting point, the JC model was defined through UHARD user subroutine. The intermediate state in the MIS method is defined according to the melting, re-melting, and relaxation process of the point of interest at the bottom layer. The layer thickness and process parameters are determining factors in this situation. Since the speed of depositions is very fast, the time step associated with the intermediate state for all points of interest in the concerned layer can be defined as long as this layer is partially re-melted by the subsequent layers. Then, the related

time step at which the final uppermost layer is completely deposited, resulting in the re-melting of the layer of interest, can be specified as the intermediate time step to extract elastic and plastic strains.

Table 3.3 Process-modeling parameters used in the microscale

Process parameters	Values
Heat source dimension $a_f = a_r = a$ (μm)	40
Heat source dimension b (μm)	40
Heat source dimension, depth c (μm)	45
Hatching space (μm)	140
Laser absorption coefficient (α)	0.55
Recoating time between two layers (s)	10

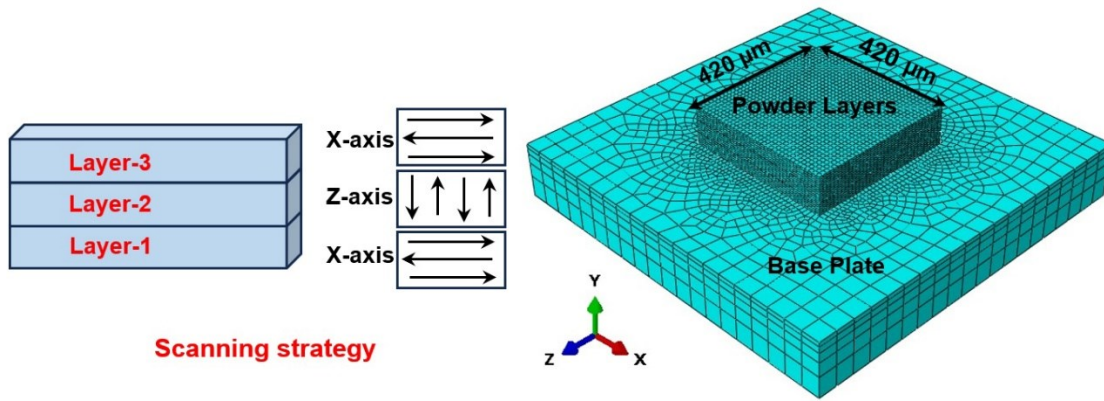


Fig 3.7 Computational domain and the scanning pattern for microscale modeling

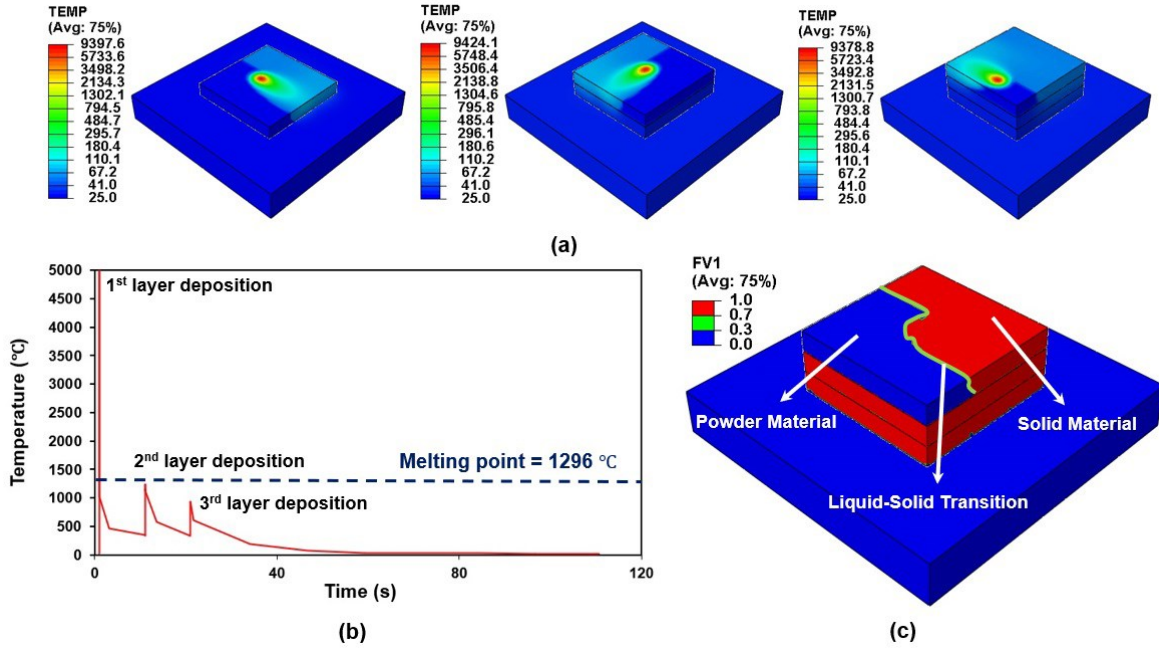


Fig 3.8 (a) Rotational scanning path of each layer, (b) temperature history of a selected point at the 1st layer, (c) defined field variable (FV1) to account for the transition from powder to solid phase

3.3.3.3 Part-scale modeling scheme

The quasi-static mechanical simulation at the part-scale is performed on a single cantilever beam (AMBench2018 challenge proposed by NIST [120]). The mean inherent strain vectors from the microscale are applied as the initial thermal strains layer by layer to predict the residual stresses and distortions. Different numbers of physical layers are merged together (layer agglomeration) to accelerate the computational time, and the elements are activated sequentially, one layer at a time. According to the literature [27], a specific number of equivalent layers needs to be identified to speed up the non-linear simulation while maintaining the accuracy. In this step, the influence of material plasticity behaviors on the number of equivalent layers is also investigated. The computational domain and geometry of printed components are illustrated in Fig 3.9. All the calculations were performed on a workstation with Intel(R) Xeon(R) CPU E5-2650 v2 with 16 cores and 128 GB RAM. To experimentally validate the modeling, the cantilever beams were printed by RENISHAW AM 400 LPBF machine. Once the built of cantilever was finished, the support structure was cut off from 3 mm above the substrate alongside the red dashed line and the beam bent upward due to the release of the residual stress (Fig 3.10). The optical scan deformation analysis was performed before and after support removal.

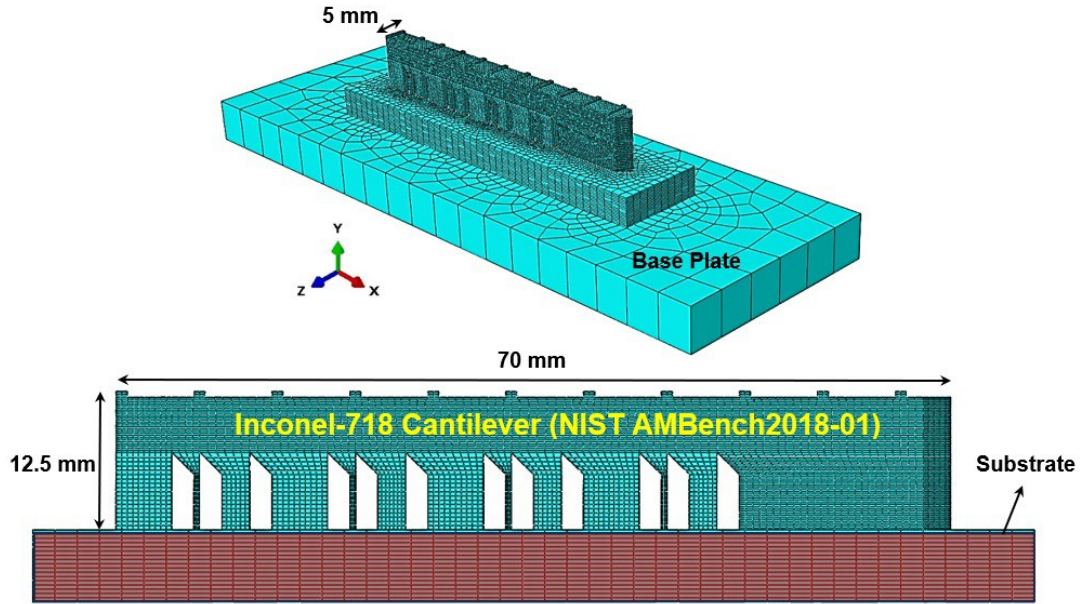
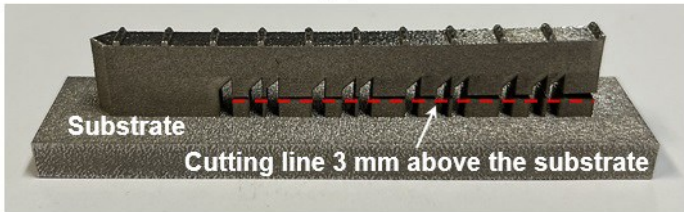


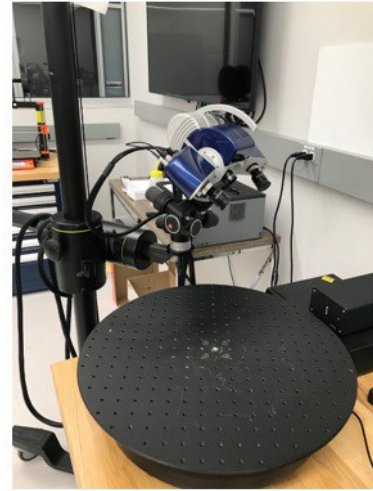
Fig 3.9 Computational domain and geometry of the NIST AMBench2018-01 [120]



(a)



(b)



(c)

Fig 3.10 a) Cantilever beams printed by RENISHAW AM 400 LPBF machine. (b) Cantilever beam after support removal; (c) optical scan deformation analyzer

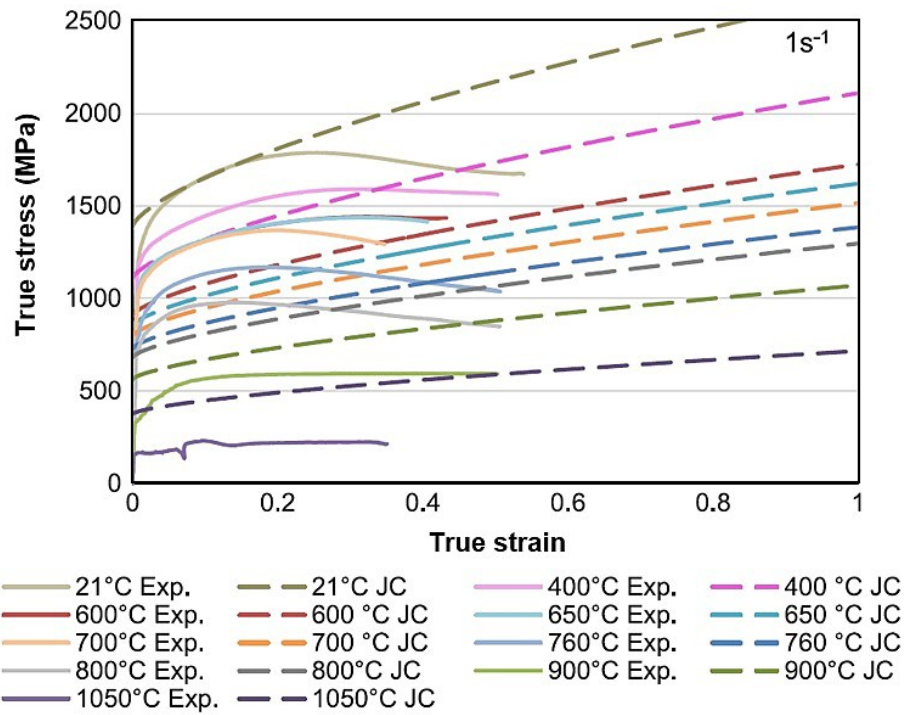
3.4 Results and Discussion

3.4.1 Mean inherent strain vectors

After performing the detailed thermo-mechanical simulation, the inherent strain values provided in Table 3.4 were extracted for four different material models (elastic-perfectly plastic (EPP), Johnson-Cook (JC), isotropic hardening (IsoH), and kinematic hardening (KinH)). The results for Inconel-718 show that the order of average inherent strain values is $\varepsilon_{EPP} \geq \varepsilon_{JC} > \varepsilon_{KinH} > \varepsilon_{IsoH}$. These results are reasonable since the IsoH, KinH, and JC models compared to the EPP, are subjected to lower plastic strain beyond the yield point under similar thermal load, respectively. Moreover, under cyclic loading, IsoH underestimates the strain values compared with the KinH. To further verify this observation, a plate featuring a circular hole as shown in **Error! Reference source not found.** in Appendix A, was subjected to a thermo-mechanical low cycle fatigue analysis in accordance with the DNV-RP-C208 [121]. The hysteresis diagram for the IsoH and KinH material models was then extracted (Fig 3.21 in Appendix 3B). Examination of results reveals that higher strains were induced by the KinH under identical loading conditions. Although the JC model is a type of IsoH that considers the rate of hardening and thermal softening, the IS values are almost the same as the EPP model. As reported in the literature [117], it has been shown that in the JC model, the level of stress exhibits a linear decline in response to an increase in temperature, which corresponds directly with the parameter, m , one of the material constants in the JC plasticity model. This estimation significantly underestimates the mechanical properties of Inconel-718 at temperatures below 900 °C, while it overestimates the stress levels beyond this temperature threshold as shown in Fig 3.11. Therefore, the JC model cannot provide a reliable estimation of IS values. One possible solution is to investigate the modified-JC model [117] as an alternative method to address the underestimated mechanical properties observed in the original JC model which may be addressed in future research study. The IS values in the x (longitudinal) and z (transverse) directions are compressive whereas the through the build direction (y) ones are tensile type. There was a slightly lower magnitude of inherent strain in the direction of laser scanning compared to the transverse direction, likely due to the 90° rotational scanning in two consecutive layers. However, previous research has demonstrated that in-layer inherent strains tend to be consistent regardless of the actual rotation angle when the laser scanning path rotates periodically [26]. Thus, a consistent value for the in-layer plane was obtained by averaging the inherent strain values in the x and z directions.

Table 3.4 Inherent strains values for different material plasticity behaviors

Material Plasticity Model	Inherent strain values		
	ε_{xx}	ε_{yy}	ε_{zz}
Elastic-Perfectly Plastic (EPP)	-0.002	0.003	-0.002
Kinematic Hardening (KinH)	-0.0017	0.0026	-0.0017
Johnson-Cook (JC)	-0.002	0.003	-0.002
Isotropic Hardening (IsoH)	-0.0015	0.002	-0.0015

**Fig 3.11** Comparisons between the temperature-dependent experimental and predicted results with the JC model in Inconel-718 at the strain rate of 1 s⁻¹[117]

3.4.2 Single cantilever residual stress and distortion

3.4.2.1 Residual distortion

Fig 3.12 illustrates the concurrent analysis of the effects of the number of equivalent layers and material models on the total distortion. The findings reveal that the KinH material model demonstrates a superior capability to yield more precise results when compared to alternative material models. Notably, the outcomes suggest that not only does the KinH yield total distortions that closely align with experimental observations, but it also allows for the utilization of a smaller

number of equivalent layers in contrast to other material models. This reduction in equivalent layers has the potential to lead to a noteworthy decrease in computational time. Examination of results also reveal that EPP model overestimates the total distortions while the IsoH underestimates the distortions compared to the experiment. The smaller magnitude of IS values on the one hand, and the influence of layer-by-layer cyclic loading on the other hand contribute to the underestimation of IsoH. Table 3.5 illustrates the correlation between the number of agglomerated physical layers and the total number of equivalent layers.

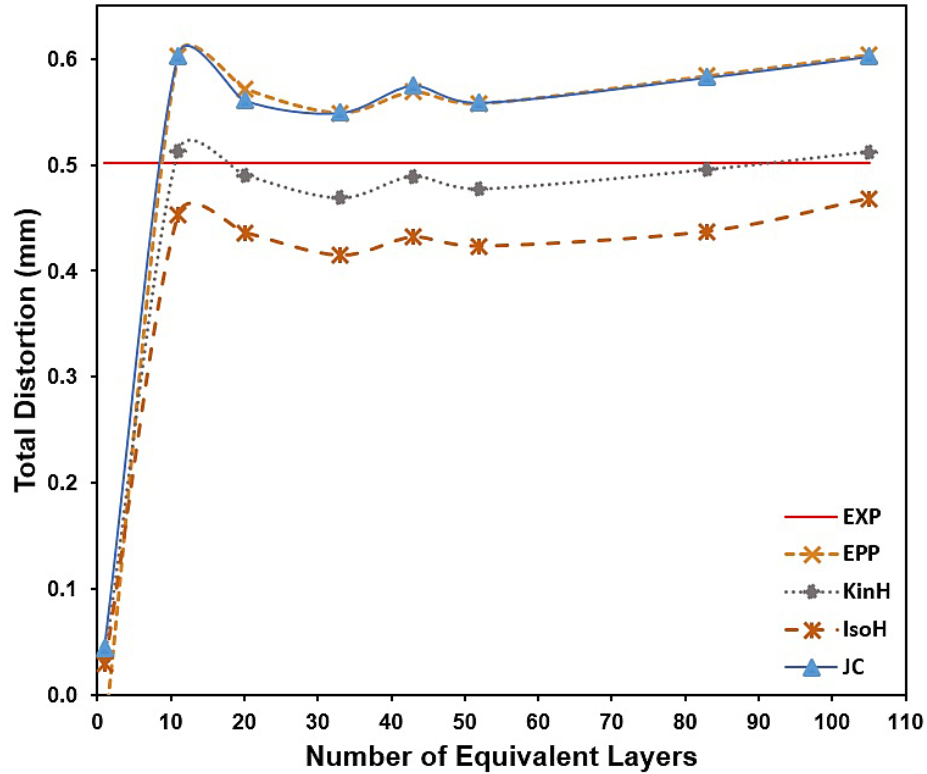
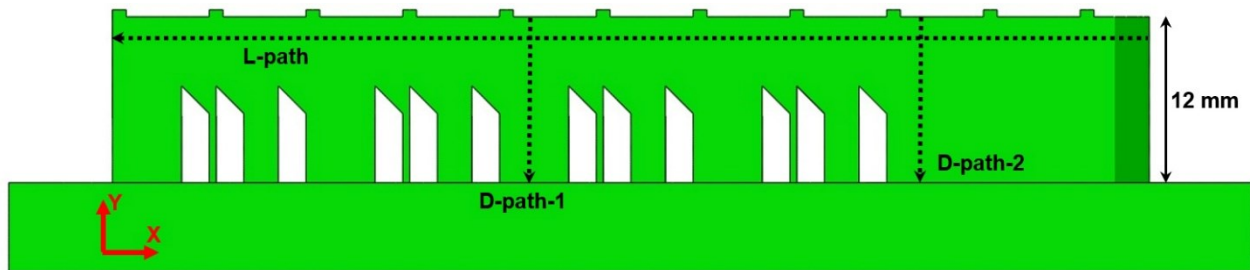


Fig 3.12 Maximum total distortion after stress relaxation of the cantilever beam containing varying number of equivalent layers, through the experiment and different material models

Results suggest that for all material models, one equivalent layer modeling yields the worst-case scenario with negligible residual stress in the top portion of the beam, leading to the smallest overall distortion. There is a sharp increase in the amount of total distortion as the number of equivalent layers is increased to 10 as shown in Fig 3.12. In this scenario, depositing a thick layer over a layer with fewer lumping generates substantial stress along the cutting line. The reduction in the number of equivalent layers basically diminishes the discernible influence of the relaxation effect on stress at the specific interface. This is completely in accordance with the findings in [27].

Results show that by increasing the number of equivalent layers above 10, JC and EPP models provide the same trend and generally overestimates the total distortion while KinH and IsoH models underestimate it. The KinH and IsoH models, however, overestimate the total distortion when the number of equivalent layers increases beyond 83 and 110, respectively. The potential reason for this phenomenon is related to the progressive accumulation of initial strain on a layer-by-layer basis, resulting in the inability of stress relaxation to overcome cyclic loading. Fig 3.13 illustrates the variation of the normal residual stress S_{11}, S_{22} throughout the depth or build direction (D-path-1) for varying numbers of equivalent layers, in accordance with the KinH model. Results show that as the number of equivalent layers increases beyond 60, a higher magnitude of tensile stress, S_{11} , is accumulated in the upper layers. In addition, greater compressive stress, S_{22} , is generated for the 83 and 105 equivalent layers, leading to additional deformation. Similar behavior is observed in other material plasticity models. As a result, to make sure that the predictions made by the layer-by-layer modeling are accurate and computationally efficient, the number of equivalent layers must fall within an appropriate limit (from 20 to 52) in which the total deformation is insensitive to the number of equivalent layers. To compare the part distortion predicted using various material plasticity behaviors with that of experiment, the nodal displacement of the presentative ridge (R_i) points at the top surface of the cantilever, as shown in Fig 3.14, along the build direction is evaluated for 43 equivalent layers. Results show that the KinH exhibits a high degree of agreement with the experiment, with an average error under 3%. The EPP and JC models exhibit a high degree of similarity, as they both tend to overestimate the displacement. On the other hand, the IsoH model typically underestimates the nodal translation in comparison to the experimental results.



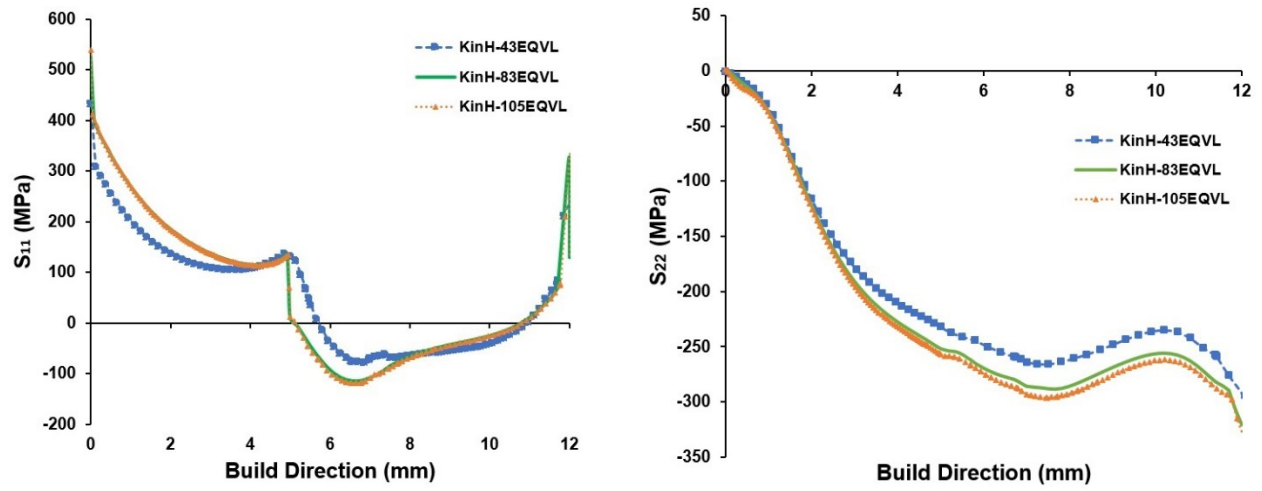


Fig 3.13 Variation of the residual stress S_{11} , S_{22} throughout the depth direction (D-path-1) for different number of equivalent layers (EQVL)

Table 3.5 Number of agglomerated physical layers associated with the total number of equivalent layers

Number of equivalent layers (EQVL)	1	10	20	33	43	52	60	83	105
Number of real physical layers that are lumped together as one layer	200	20	10	6	5	4	3.5	2.5	2

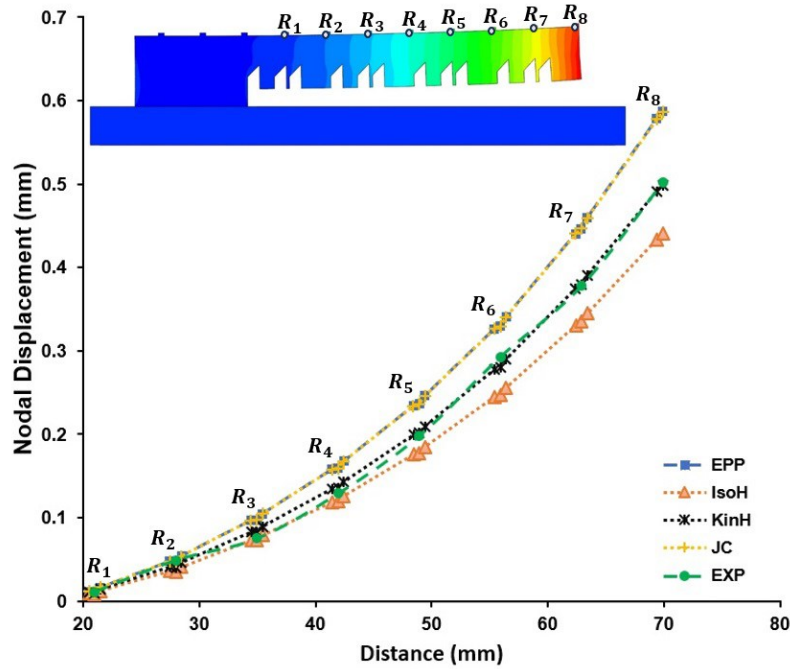


Fig 3.14 Nodal displacement validation with experiment for various material models and 43 equivalent layers

3.4.2.2 Residual stress

The predicted von Mises stress distribution of the 43 equivalent layers cantilever beam prior to and after the removal of the support structure from the substrate is shown in Fig 3.15 for the KinH model as an example. The von Mises stress generally exceeds the yield strength of the material, implying the occurrence of plastic deformation at the end of the process for all material models. The initial cut from the base plate causes the highest stress at the bottom of the substrate. Before the removal of the cantilever support from the substrate, the left and right sides of the connection between the cantilever beam and substrate experience the maximum von Mises stress. Furthermore, the von Mises stress through the thickness is minimum in the center of the beam and increases near the top and side surfaces. The order of average von Mises stress in the cantilever beam for all material models is found to be $\sigma_{EPP} = 505 \text{ MPa} \geq \sigma_{JC} = 500 \text{ MPa} > \sigma_{KinH} = 433 \text{ MPa} > \sigma_{IsoH} = 383 \text{ MPa}$. These results are reasonable because the KinH and IsoH provide higher yield strength due to the hardening effect and reach the yield point later under the same loading condition compared to the EPP model. As discussed earlier, the JC model overestimates the residual stress at room temperature. Although the highest values of JC parameters were chosen from the literature to compensate for the yield strength underestimation, the model cannot predict the real residual stress resulting from the hardening and rate of hardening effects. Upon removing the support, a portion of the stress is relieved at the connection between the substrate and the cantilever beam. This leads to a decrease in the maximum von Mises stress for all material models and causes the cantilever beam to bend upwards in the build-up direction. The stress components contour for the KinH model with 43 equivalent layers as an example is shown in Fig 3.16 before the support removal. The greatest magnitude of longitudinal tensile residual stress S_{11} is located at the lower layers of the cantilever, while compressive stress is observed in the intermediate section of the component. The tensile stress in the uppermost depositions results from the contraction of the molten material during solidification. The residual stress S_{22} along the build direction is mainly compressive at all points except the side surfaces of cantilever beam. It is evident that the maximum value of S_{22} , found at the boundary of the cantilever and substrate, which is lower than the material yield point (1170 MPa) except a very infinitesimal region at the right end point. This indicates that there is no delamination happening. The transverse residual stress S_{33} is relatively compressive in the middle section and becomes tensile in the top layer.

Following the detachment of support, the residual stresses in all directions are released, resulting in mostly compressive stresses in the central region, as seen in Fig 3.17.

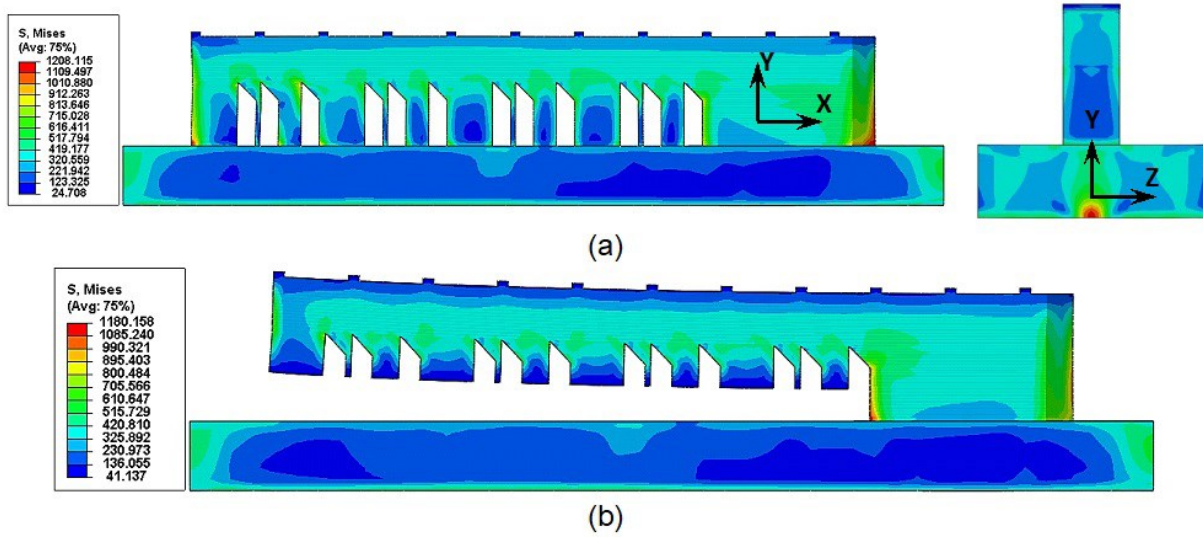
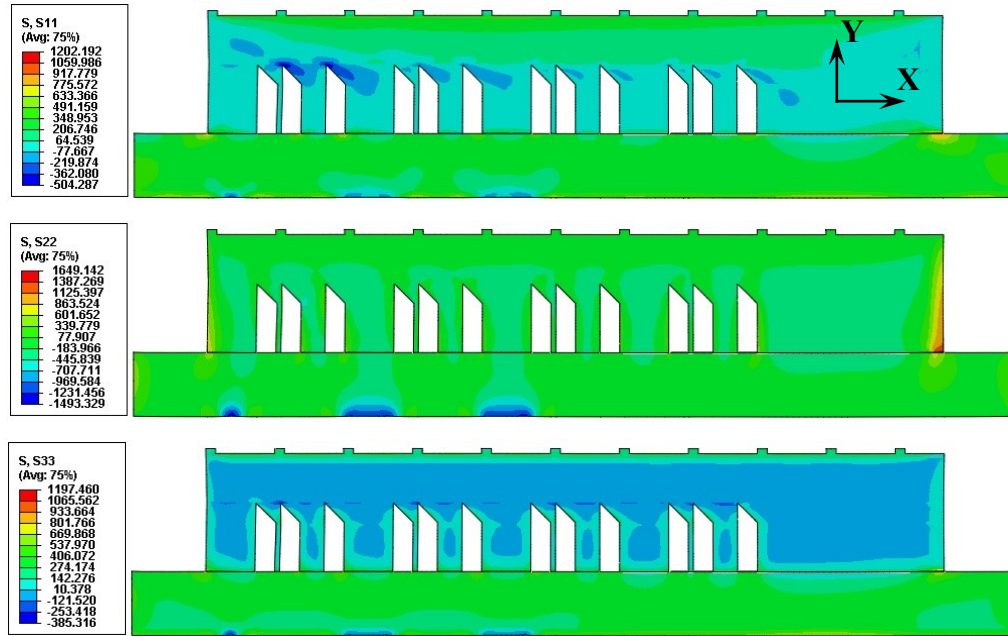
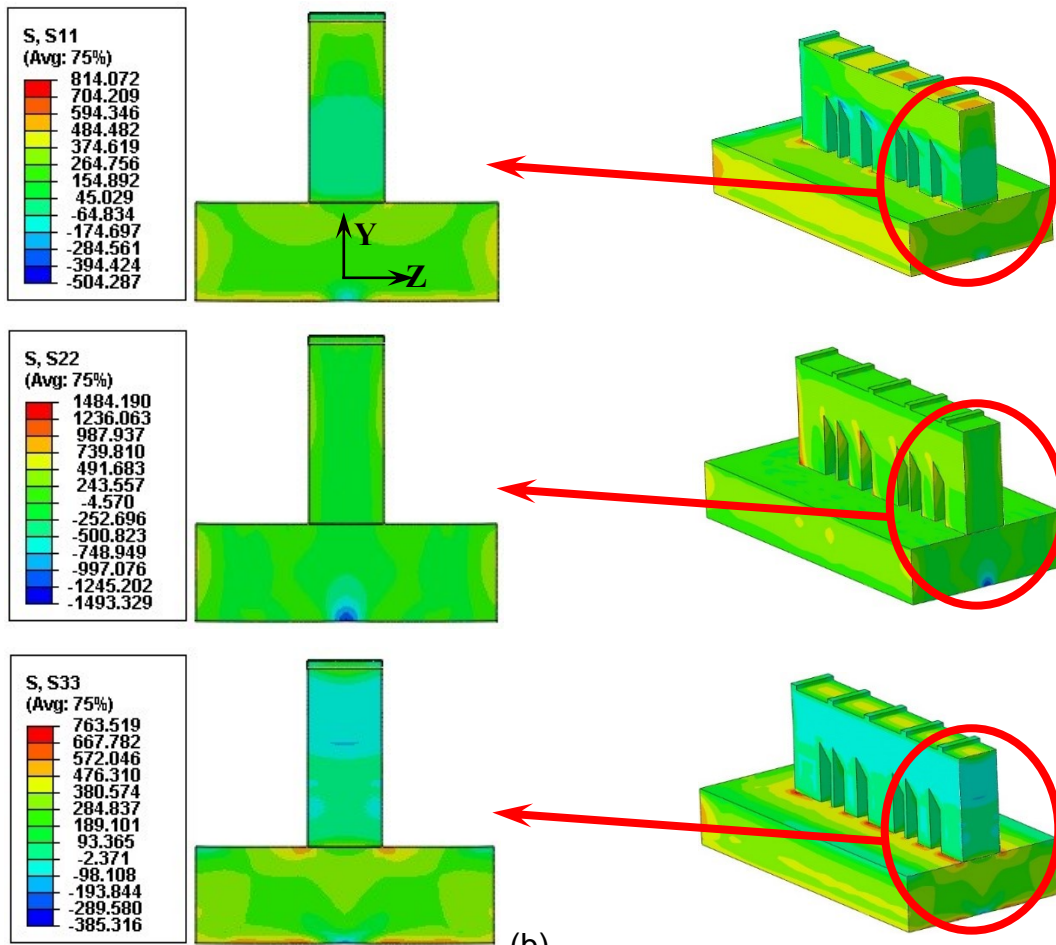


Fig 3.15 Von Mises residual stress contours a) before and b) after support removal for KinH model

Fig 3.18 presents a comparative analysis of the variation in residual stress components across various material models before and after the removal of the support, in both the longitudinal (L-path), close to the top surface, and depth (D-path-2) directions for 43 equivalent layers. The L-path and D-path-2 are previously illustrated in Fig 3.13. The D-path-2 was selected since it is not possible to evaluate the residual stress along D-path-1 after the support removal. The normal residual stress S_{11} has the following order of magnitude $S_{11-EPP} \geq S_{11-JC} > S_{11-KinH} > S_{11-IsoH}$ along the L-path before the support removal and it dramatically decreases to around -20 MPa (compressive) for all material models when the support is removed (Fig 3.18(a)). The stress fluctuation at both left and right ends is a consequence of edge boundary conditions. The S_{11} stress component along the D-path-2 has an identical order of magnitude to its L-path before cutting the support for various material models as shown in Fig 3.18(b). The stress profile decreases gradually until the midpoint, followed by a slight increase towards the bottom of the cantilever. Previous studies also demonstrated a similar pattern for the S_{11} profile both experimentally and numerically [62,122]. Following the support removal, the residual stress S_{11} along the D-path-2 is released in the top layers and transforms into a compressive state for all material behaviors. The residual stress S_{22} along the L-path remains consistently at around -15 MPa for all material models, both before and after the support separation as shown in Fig 3.18(c).



(a)



(b)

Fig 3.16 Residual stress contours for KinH model before cutting support along the longitudinal (S_{11}), depth (S_{22}), and transverse (S_{33}) directions on a) XY plane, b) YZ plane

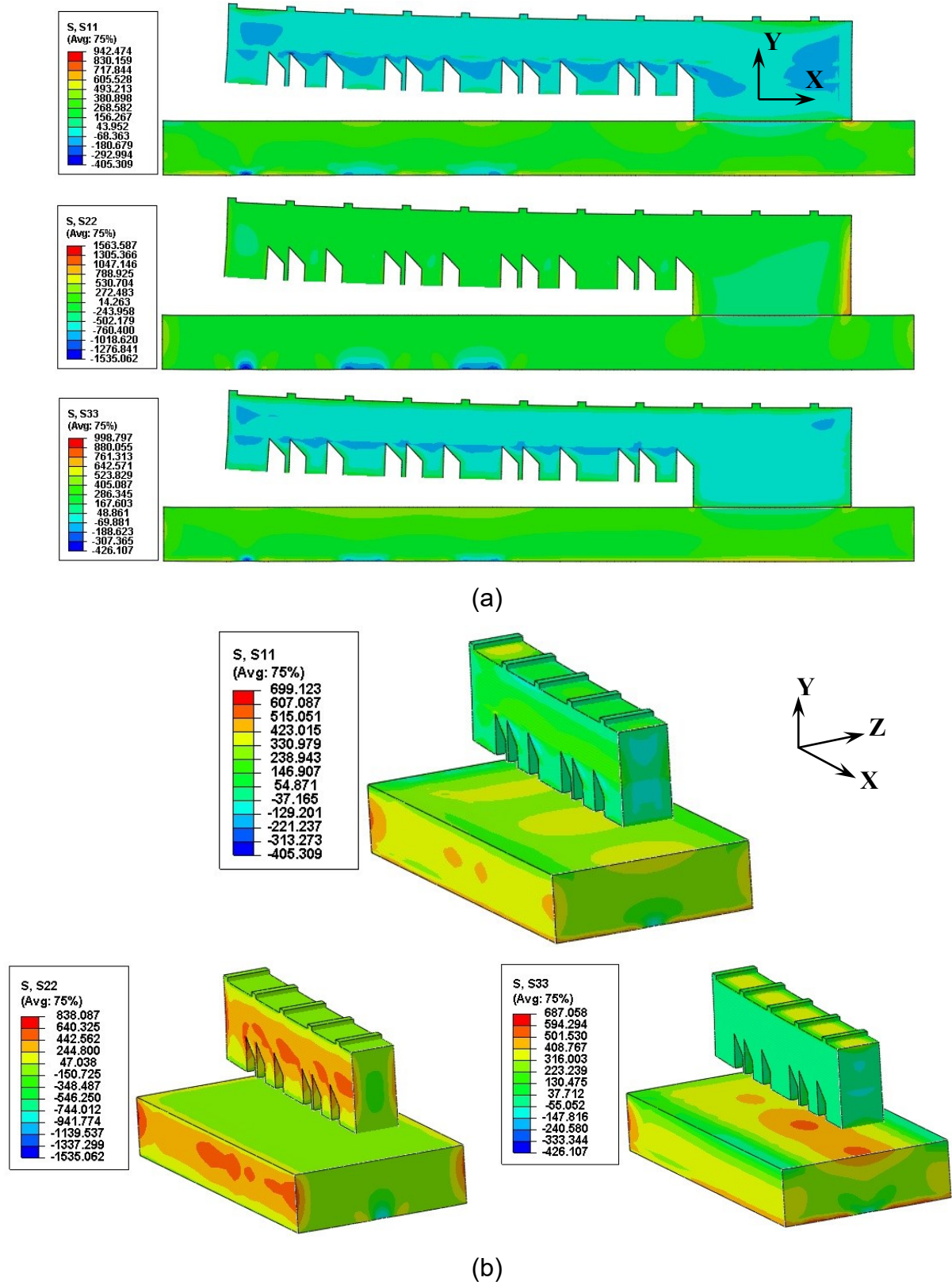
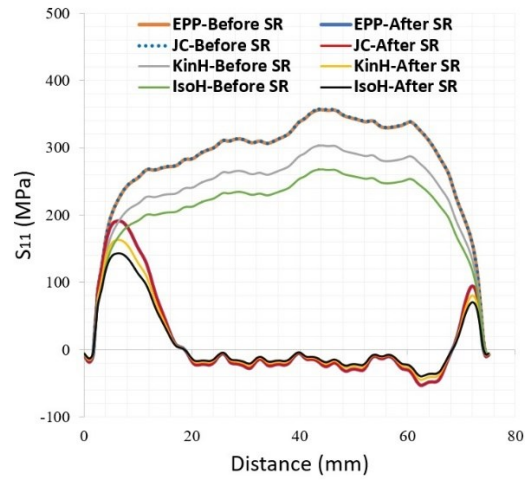
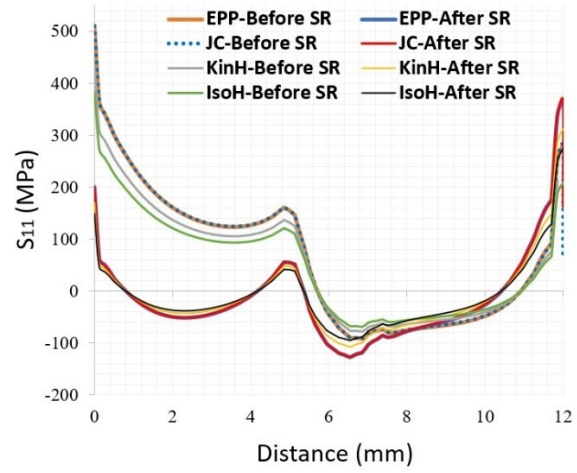


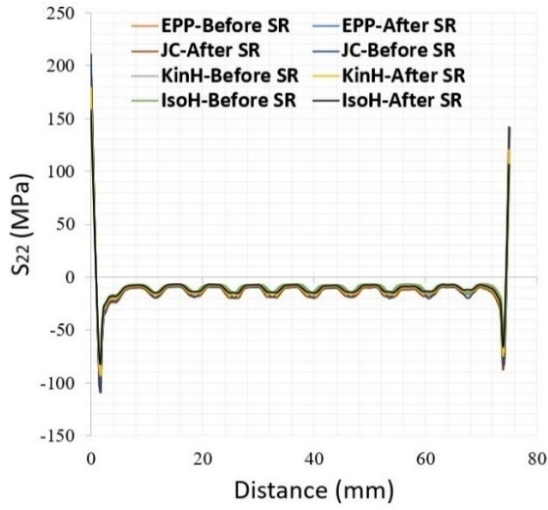
Fig 3.17 Residual stress contours for KinH model after cutting support along the longitudinal (S_{11}), depth (S_{22}), and transverse (S_{33}) directions on a) XY plane, b) isometric view



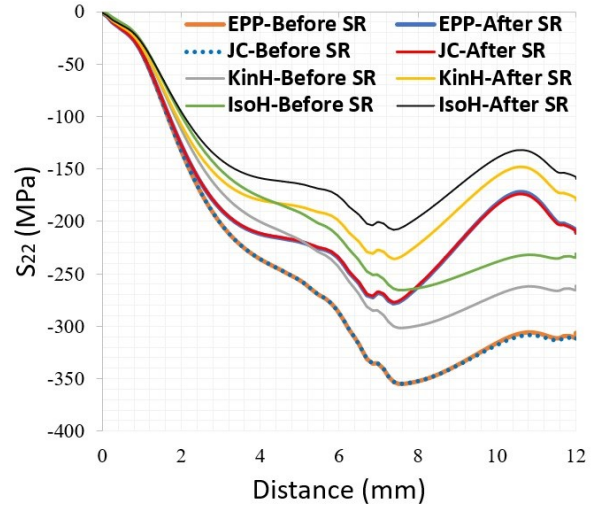
(a)



(b)



(c)



(d)

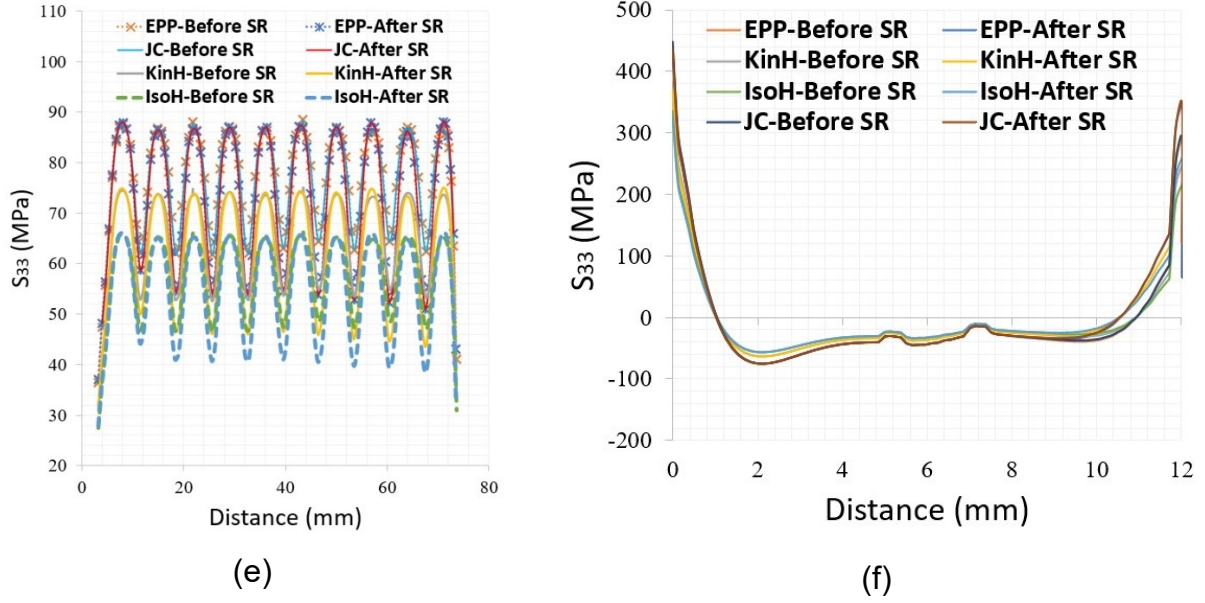


Fig 3.18 Comparison of residual stress components before and after the support removal (SR) for various material models along the L-path (a, c, and e), and D-path-2 (b, d, and f) directions

On the other hand, S_{22} along the D-path-2 is completely compressive before and after the support removal with a magnitude of zero on the top layer and the following order of magnitude for various material models as $S_{22-EPP} \geq S_{22-JC} > S_{22-KinH} > S_{22-IsoH}$ at lower layers (Fig 3.18(d)). The transverse residual stress S_{33} along the L-path is completely tensile for all material models. The amount of variation between the pre- and post-cutting support is negligible for each material model (Fig 3.18(e)). This stress component along the D-path-2 is, however, compressive and is almost unaffected by the material model, as can be seen in Fig 3.18(f). The residual stress profiles depicted in Fig 3.18 demonstrate that the magnitudes of S_{11} in both directions are pivotal factors controlling the distortion of the cantilever for all material plasticity models. This observation aligns with the experimental findings reported in the literature [59,62]. In addition, the compressive stress is found to increase along the D-path-2 direction which has also been observed in [80].

3.5 Conclusion

This research presents a multi-scale thermo-mechanical model featuring the IS method. The purpose is to investigate how different material constitutive laws affect the induced IS values and the final distortion of a part manufactured by the LPBF process. Four different material plasticity models were used, namely, elastic-perfectly plastic (EPP), Johnson-Cook (JC), isotropic hardening (IsoH), and kinematic hardening (KinH). The thermal analysis was performed on the microscale,

and the temperature distribution was applied as the thermal load in the static analysis. The IS values were subsequently extracted from a 3-layer microscale representative for Inconel-718 and applied as the initial strains to the part-scale in a layer-by-layer quasi-static simulation. The cantilever beam as a complex part-scale model was used to examine the accuracy of the proposed models with experiment according to the number of equivalent layers in the agglomeration approach. Key findings are summarized as follows:

- The utilization of four distinct material models yields varying IS values when subjected to similar process parameters. The IsoH and KinH obtained the smallest IS values, respectively, as a result of the hardening effect. The magnitude of the IS values is overestimated by the JC model, which is almost equivalent to the EPP model.
- The accuracy of the prediction for different material models was investigated by altering the number of equivalent layers in the part-scale simulation. The KinH model was able to provide more accurate predictions compared to competing material models with an error of less than 6 % for the number of equivalent layers in the range of 20 to 52. Moreover, it enables the implementation of a smaller number of equivalent layers when compared to alternative material models. The potential consequence of this reduction in equivalent layers is a significant decrease in computational time.
- The IsoH underestimates the total distortion due to the smaller values of IS and the impact of cyclic loading in the layer-by-layer simulation. On the other hand, the EPP and JC models overestimate the total distortion.
- Part distortion is primarily caused by the in-plane anisotropic stresses (S_{11}, S_{33}) along longitudinal direction and S_{22} along depth direction for all material models.
- Prior to support removal, a substantial tensile residual stress along the longitudinal direction was predicted on the uppermost layers of the cantilever. After the support was removed, the tensile residual stress in the uppermost layers dropped by over 100 % and it became compressive for all material models.
- The choice of material may significantly influence the amount of tensile residual stress near the top surface, leading to a more accurate prediction of total distortion when compared to the experimental data. Following the elimination of support, all material

models converge to almost identical values of longitudinal residual stress S_{11} along the laser scanning and build directions.

- The present study revealed the importance of hardening effect to enhance the accuracy of the prediction in the IS method for a complex part. Since the JC model could not predict the real distortion, the modified-JC model [117] can be implemented in future studies to account for the rate of hardening examination in final distortion. Therefore, identification of the best material model for residual distortion prediction can stimulate future studies to establish advanced artificial neural network model combined with process parameter optimization to achieve an accurate and very fast prediction.

Appendix 3A Multi-scale modeling scheme in MIS method

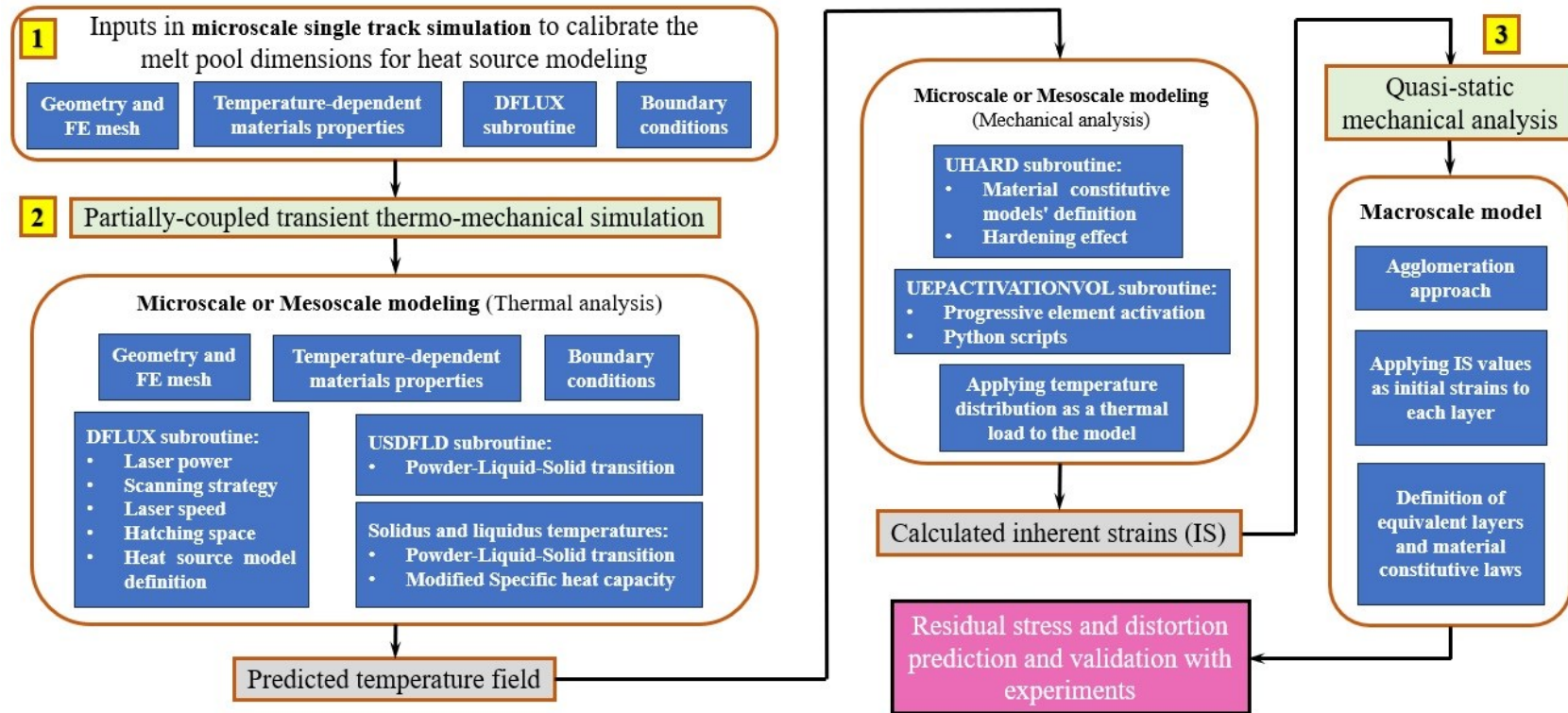


Fig 3.19 Overview of the entire multi-scale modeling scheme in the MIS method

Appendix 3B Cyclic displacement 8 mm at constant temperature 1100 °C

The finite element analysis was performed with 8-noded shell elements with reduced integration (S8R). The boundary conditions and cyclic displacement are applied as illustrated in Fig 3.20 below. It is noted that a total of 6 complete load cycles was specified in the analysis in order to see how the stress strain hysteresis curve developed (Fig 3.21).

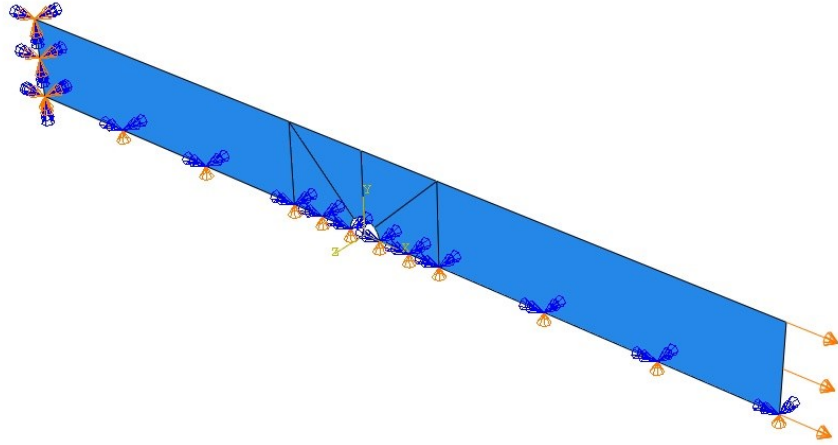


Fig 3.20 Geometry and boundary conditions

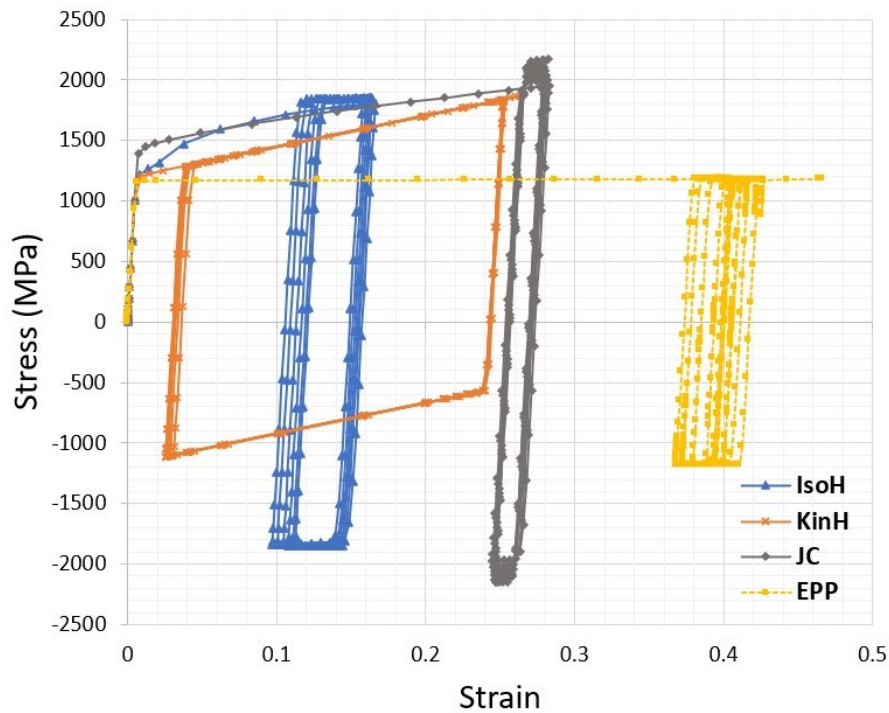


Fig 3.21 Hysteresis diagram for different material models

Chapter 4 A detailed investigation of induced residual stresses in the laser powder bed fusion process using the modified inherent strain approach and experimental measurements

Abstract: In this work, a multi-scale finite element model is proposed to simulate the Laser Powder Bed Fusion (LPBF) process, employing the Modified Inherent Strain (MIS) methodology. MIS is a more sophisticated approach than the conventional Inherent Strain (IS) technique, initially developed for welding process simulations. Due to the complicated thermo-mechanical interactions present in the metal Additive Manufacturing (AM) process, the MIS approach has evolved to deal with it, in which sequentially deposited layers act as mechanical constraints on earlier layers, influencing stress and strain evolution throughout the process. A multi-scale modeling approach can effectively predict the residual stresses induced during LPBF, which are essential for assessing the quality and performance of the manufactured part. This study provides a novel contribution by systematically validating MIS-based residual stress predictions against depth-resolved X-ray diffraction (XRD) measurements up to 3 mm below the surface, addressing a critical gap in the literature where prior works primarily focused on surface-level stress or distortion. Laser power and velocity, which are critical process parameters, were modified to investigate their individual impacts on the residual stress distribution in the longitudinal and transverse directions. Simulated results were validated through experimental XRD measurements on fabricated Inconel-625 test coupons. While the MIS method aligns well with the experimental data at the surface level, discrepancies arise in deeper subsurface layers, where simulations tend to underestimate tensile residual stresses. This indicates that additional refinement, such as thermal-microstructural coupling, may be necessary to enhance stress prediction accuracy in multi-layer AM processes. By offering a comprehensive depth-resolved analysis, this work provides new insights into subsurface stress evolution, critical for ensuring the structural integrity of LPBF parts. The study provides a critical assessment of the MIS method's capabilities and provide essential guidance for future research opportunities to improve residual stress predictions in LPBF-produced parts.

4.1 Introduction

Additive manufacturing has emerged as a revolutionary technique that enables the fabrication of complex shapes directly from digital designs [123]. Among the various AM techniques, LPBF has gained significant attention across various industries, particularly in aerospace, automotive, and biomedical sectors, due to its unique capability to fabricate metal components with intricate designs, high precision, and excellent material properties [124]. However, despite these advantages, LPBF faces several challenges, particularly the generation of induced residual stresses, which may result in the ultimate product warping, flaking, and deformation in the final product [125]. Eventually, these flaws might influence the dimensional accuracy and mechanical performance of the part. The generation of residual stresses in LPBF is influenced by a wide range of factors, including material properties, part geometry, and the complex interplay of multiple process parameters such as laser power, scanning speed, hatch spacing, and layer thickness [126].

Current industrial practices primarily rely on trial-and-error methods to optimize these parameters [127]. Typically, simple geometrical samples such as cylinders and cuboids are used during the optimization phase. However, the parameters that are optimized for these basic shapes often fail to perform adequately in more complex geometries. For example, features like sharp corners, edges, holes, internal channels, complex internal structures, overhangs, and thin walls cause uneven heat dissipation, leading to temperature gradients, microstructural variations, and consequently residual stresses, cracking, and distortion [127–132]. Consequently, the process of optimizing parameters for new designs is not only time-consuming but also resource-intensive, often requiring months of iterative testing [45,119,122,133]. To overcome these challenges, there is a pressing need to develop physics-based models capable of accurately predicting defects across various scales, ranging from microscale (Fig 4.1 (a) [131,133]), where porosities emerge (Fig 4.1 (b) [122]), to the mesoscale (Fig 4.1 (c) [131]), where sintering behavior, bonding properties between successive melt track layers and the formation of process-related metallurgical defects [134] are modeled (Fig 4.1 (d) [135]). At the macroscale (Fig 4.1 (e) [136]), simulations address fracture and cracking (Fig 4.1 (f) [16]) driven by residual stresses. By leveraging advanced multi-physics simulation techniques, these defects can be predicted and mitigated before they compromise the integrity of the final product [23,81,104,131,136–138].

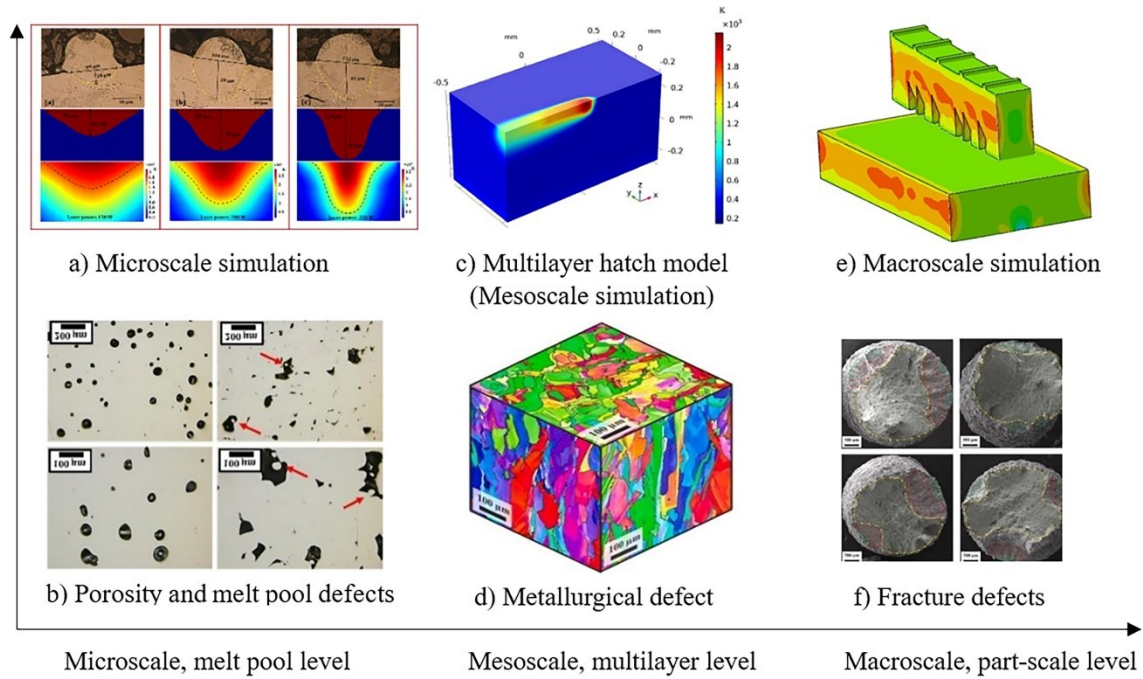


Fig 4.1 Defects across various scales and physics-based multi-scale simulation of LPBF process

4.1.1 Recent advanced strategies for multi-scale modeling in LPBF

Various strategies have been developed and investigated to tackle the challenges of predicting part-scale phenomena in LPBF, with an emphasis on methods that balance accuracy and computational efficiency [119,128,143–147,132,133,136,138–142]. Computational methods, such as Finite Element (FE), Lattice Boltzmann, Finite Volume, and discrete element methods are effectively employed to study microscale phenomena, offering detailed insights into localized heat and material interactions, critical for part quality at fine scales [148–151].

At the microscale, simulations focus on key phenomena such as heat transfer (including convection, conduction, and radiation), evaporation, recoil pressure, cooling, solidification, and laser-material interactions [152]. Research has extensively explored these microscale behaviors, often integrating several or all these phenomena into simulations efficiency [128,132,133,136]. Capillary forces, driven by surface tension inside the melt pool, are essential in contouring the melt pool, enhancing stability, and improving wettability, which in turn reduces porosity and increases the final product's density [153]. Additionally, capillary forces induce Marangoni convection, which facilitates improved heat distribution and more uniform melting. Recoil pressure, generated

by vapor in the high-energy melt pool, can introduce pores when the vapor collapses as surface tension overpowers the recoil pressure during cooling [153].

A key factor in the success of LPBF simulations is the accurate modeling of heat distribution within the heat-affected zone, achieved through advanced heat source models. These models are essential for making reliable predictions about residual stresses and distortions. However, directly applying detailed microscale models to part-scale simulations presents significant computational challenges. The sheer complexity and scale of part-scale simulations make it impractical to rely on microscale methods alone due to the vast computational resources required.

To address the limitations of relying solely on microscale simulations, multi-scale simulation approaches have been subsequently developed. These approaches seamlessly integrate microscale and mesoscale models with part-scale (macroscale) simulations, providing a more holistic analysis of the LPBF process [65,134]. By incorporating these multiple scales, researchers can better predict how localized phenomena, such as porosity and thermal gradients, influence the overall geometry and structural integrity of the final part. These methods combine the detailed precision of microscale models with the broader scope of part-scale simulations, enabling accurate predictions of distortion and residual stresses without overwhelming computational resources.

In multi-scale simulation, the temperature distribution derived from a mesoscale thermal simulation or an equivalent heat source (thermal model/lumping) [154], is used in a subsequent macroscale thermo-mechanical simulation [140]. Alternatively, inherent strain values from a thermo-mechanical mesoscale analysis can be applied to a purely mechanical macroscale simulation [23,134,136,146]. Each of these methods (thermal model/lumping and inherent strain) offers unique advantages in managing the complexity of multi-scale simulations, particularly when attempting to scale up from microscale to part-scale simulations. Fig 4.2 illustrates the sequential analysis procedure for multi-scale modeling. The bullet point types at mesoscale and macroscale are linked together.

4.1.1.1 Lumping and thermo-mechanical models

Thermal modeling plays a crucial role in LPBF simulations by predicting temperature distributions and thermal histories throughout the build process. To simplify these simulations, researchers have extensively investigated various solutions, such as lumping, which involves combining several layers into a single, thicker layer [119,132,139,140]. This method reduces the number of layers

that need to be simulated, thereby decreasing computational time. Zaeh and Branner [62] developed a FE model using layer lumping to calculate the residual stress of the printed cantilever beams, which was subsequently verified through neutron diffractometry experiments. This approach efficiently manages thermal gradients and residual stresses but may sacrifice some detail in localized temperature profiles. Another effective methodology to enhance simulation efficiency is enlarging heat source dimensions and merging several layers. Promopattum et al. [130] implemented a layer fashion thermal input methodology to predict temperature gradient in macroscale LPBF parts. Li et al. [122] calculated the distortion of twin cantilever beams produced by LPBF through a multi-scale model technic [65,122]. In this method, the local residual stresses were determined first by applying the equivalent heat source obtained from microscale model to the hatch model. Then, the results were mapped to the macroscale model to predict the residual distortion of the printed parts. Further advancements by Li et al. [65] included enlarging their macroscale model which allowed them to use greater layer thickness and heat source dimensions to enhance computational efficiency. This approach was tested on bridge and L-shaped structures to predict residual stress and distortion in macroscale models. Papadakis and Papadakis et al. [155] utilized volume-based heat input in the part-scale modeling to speed up the simulation process, achieving results close to those obtained by Zaeh and Branner [62]. Bonakdar et al. [154] developed a Gaussian effective heat flux model tailored for line-type irradiation scans, where the heat source parameters and the thermal conductivity coefficient are calibrated for macroscale applications. This model, known for its efficiency and precision, significantly reduces computational costs [139,154]. While strategies such as lumping, enlarging heat source dimensions or using effective heat flux models, can effectively speed up simulations, they often fail to accurately capture localized temperature variations and cooling rates. Moreover, attempting to introduce a moving heat source that accurately represents the scanning strategy into a thermo-mechanical simulation can greatly increase computational costs. This is because the simulation needs to continuously adapt to the changing heat distribution as the laser moves, which is computationally intensive. Therefore, while these methods offer efficiency gains, they also come with trade-offs in accuracy and flexibility, particularly when trying to model the real-time dynamics of LPBF process.

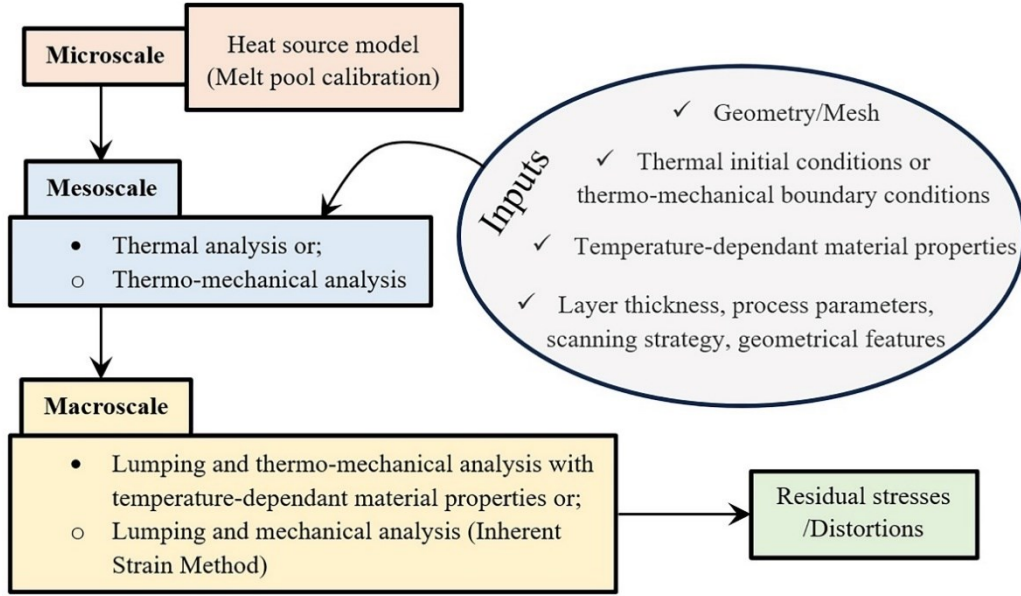


Fig 4.2 The procedure of the sequential different multi-scale simulations of LPBF process

4.1.1.2 Inherent strain (IS) approach

The inherent strain approach has become a prominent method to expedite macroscale simulations in LPBF [81,137,144,146,147,156–159]. To address the significant computational challenges of LPBF simulation, a few studies have investigated the inherent strain method [15]. This approach has proven to be an effective and practical solution for predicting residual stresses and distortions. Basically, the IS approach involves three main steps: 1) Single track thermo-mechanical simulation and development of heat source model (microscale); 2) Multi-path thermo-mechanical modeling on the mesoscale to extract the thermal history and the inherent plastic strains in the steady state room temperature (hatch model); 3) Macroscale simulation of the process by applying the obtained anisotropic plastic strains to a real part geometry as the initial loads and conducting a quasi-static analysis [23,30,160]. By leveraging IS values from microscale simulations, Keller and Ploshikhin [21] significantly reduced the computational time in macroscale modeling of the LPBF. Their work demonstrated that the IS method could streamline simulations while maintaining accuracy. Liang et al. [23,27] offered and validated a modified inherent strain (MIS) approach using thin walls and rectangular contours, achieving accurate predictions of residual stress and distortion. In summary, the IS approach allows for the consideration of scanning strategies in LPBF simulations with much lower computational costs. Instead of simulating the dynamic heat input in real-time, this method pre-calculates strain fields from detailed mesoscale simulations. These inherent strains, which capture the effects of different scanning strategies, are then loaded to a macroscale model. This

simplifies the process, enabling the simulation of residual stresses and distortions across the part without the heavy computational load associated with traditional real-time methods.

4.1.2 Limitations of the multi-scale simulation techniques

Despite significant advancements in multi-scale simulation techniques, several notable limitations persist in the current practices for the residual stresses and distortions prediction in LPBF, which hinder the accuracy, efficiency, and scalability of simulations, especially when applied to complex industrial parts. One of the primary challenges is the high computational costs and scalability issues associated with thermo-mechanical modeling, particularly when using FE models. While techniques such as adaptive mesh refinement and multi-scale modeling frameworks have been developed, they have not yet sufficiently reduced computational time for large and complex components [21,62,119,131,132].

Another limitation is related to the IS method, which, although efficient in reducing computational complexity, often assumes uniform plastic strain [30]. This assumption can lead to inaccuracies, particularly in geometries that differ from the calibration sample. Additionally, this method struggles with capturing the full thermal history and the non-homogeneous nature of distortions, leading to potential errors in predicting residual stresses and deformations [23,122,161].

Thermal models and approaches that involve enlarging heat source dimensions also present challenges. Lumping, which combines multiple layers into one, often sacrifices the detailed representation of thermal gradients and transient effects, leading to less accurate predictions of localized temperature variations, phase transformations, and microstructural evolution. This issue is particularly problematic in parts with complex geometries, where oversimplification can result in unreliable predictions of residual stresses and distortions. Enlarging heat source dimensions tends to smooth out the actual, highly localized heat distribution that occurs in LPBF, leading to inaccurate modeling of thermal gradients and melt pool behavior, which are critical for predicting localized defects such as porosity and cracking. These approaches, while reducing computational time, often do so at the cost of precision, particularly in simulations where the accuracy of thermal behavior, defect formation, and stress predictions is crucial [143,155,160,162].

Over the past decade, the IS method has become widely adopted as a fast and computationally efficient approach to predict residual stresses and distortions in macroscale modeling of LPBF

[104]. Inherent strain values, which represent the summation of all inelastic strains at the final cool state of a part, are crucial for simplifying complex thermo-mechanical processes while maintaining reasonable accuracy. Building on this, Chen et al. [30] developed a state-of-the-art methodology for IS calculation (MIS method), enhancing the precision of residual distortion predictions in selective laser sintering (SLS). By incorporating the fast heating and cooling cycles characteristic of continuous deposition processes, their approach showed improvement compared with the conventional IS method, which had been designed for welding applications [21]. Later, other researchers conducted extensive studies to enhance the accuracy and efficiency of the MIS method in residual stresses and distortion prediction [31,86,90]. For example, Mohammadtaheri et al. [146] investigated the critical role of hardening effects in improving computational efficiency, particularly for predicting the behavior of complex parts. They refined the MIS method to improve both prediction accuracy and computational performance.

Further advancements have been made in multi-scale models based on the IS method, offering potential solutions to the challenges of residual stress and distortion prediction in industrial-scale AM [28,29,163]. Despite these advancements, a key research gap remains in the literature including very limited comparison between experimental data and IS-based numerical predictions, particularly in terms of residual stress distribution below the top surface of components. Existing studies, such as those by Liang et al. [23,27,31,86], Keller and Ploshikhin [21], and Chen et al. [30], primarily focus on surface stress predictions or distortion analysis, with limited validation against experimental subsurface stress measurements. For instance, Zaeh and Branner [62] validated residual stresses using neutron diffraction but focused on surface-level stresses in cantilever beams, without exploring depth-resolved profiles. Similarly, Li et al. [122] validated distortions but did not provide depth-resolved stress comparisons. To the best of our knowledge, no prior studies have directly compared IS-based or MIS-based residual stress predictions with depth-resolved experimental measurements using X-ray diffraction (XRD) up to 3 mm below the surface. This study provides a pioneering contribution by systematically validating MIS-based residual stress predictions against depth-resolved XRD measurements across longitudinal, transverse, and build directions, offering new insights into subsurface stress evolution in LPBF parts. This approach addresses a critical gap in the literature, as previous works primarily focused on surface-level stress or distortion without exploring subsurface stress distributions in such detail. This study addresses this gap by providing a comprehensive comparison of MIS-based residual

stress predictions along all principal axes (longitudinal, transverse, and build directions) at depths of 0, 1000, 2000, and 3000 μm , validated against XRD measurements. This depth-resolved validation offers a previously unexplored perspective on the accuracy of the MIS method for subsurface stress prediction, critical for ensuring the structural integrity of LPBF parts. Furthermore, no prior work has systematically investigated the influence of process parameters (laser power and scanning speed) on depth-resolved stress profiles using the MIS approach, underscoring the novelty of this study.

In this study, the MIS method is employed to simulate the residual stress distribution in LPBF-manufactured parts. A multi-scale simulation approach is formulated to model residual stress formation at different scales, from the microscale heat source model to the macroscale structural analysis. The process parameters, including laser power and scanning speed, are varied to investigate their influence on the residual stress distribution in the fabricated coupons. The simulated results are validated using experimental measurements obtained through XRD, providing a comprehensive analysis of the accuracy of the MIS method and identifying areas for further refinement in residual stress prediction for LPBF parts. The following is the outline of the paper: Section 4.2 covers the governing equations along with the material properties, while Section 4.3 explains the simulation methodology. Section 4.4 presents the experimental procedure and validation of simulation results, and finally, Section 4.5 provides a discussion of the findings, concluding with insights into future research directions.

4.2 Governing equations and material properties

This section provides a concise review of the fundamental governing equations for thermo-mechanical analysis, followed by presenting the boundary conditions and material properties defined in the LPBF modeling.

4.2.1 Heat transfer governing equations

In a coordinate system with the moving heat source along the x-direction, non-linear Fourier's equation for heat transfer at the weld joint can be written as follows:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \bar{Q}(x, y, z, t) \quad (\text{Eq 4.1})$$

where x , y , z are the coordinate axes, t is time, ρ is the material density [kg/m³], c_p is the temperature-dependent specific heat capacity [J/kgK], k is the temperature-dependent thermal conductivity [W/mK], T is the temperature [K], and $\bar{Q}$ is the internal heat generation in the material [W/m³] due to heat source intensity supplied by the laser beam and heat dissipation caused by convection and radiation. The discontinuous powder bed can be replaced with a continuum material exhibiting identical material characteristics [59]. For instance, various thermal conductivity models have been proposed to consider the impact of porosity in metallic powder [110–113]. In the LPBF process, the heat generated by the laser beam is transmitted to the peripheries of the part. Consequently, thermal conduction is a critical factor in thermal analysis. The high energy density of the laser beam generates considerable radiation from the fusion bead. The radiation on the surfaces during laser beam melting can be defined as:

$$q_{rad} = -\sigma\varepsilon (T_s^4 - T_\infty^4) \quad (\text{Eq 4.2})$$

where q_{rad} is the heat loss, ε is the heat emissivity, σ is the Stefan–Boltzman constant, T_s and T_∞ are surface and ambient temperature, respectively. In addition, the deposition layer and the surrounding powders are subjected to convection heat transfer with the environment as below:

$$q_{conv} = -h_c (T_s - T_\infty) \quad (\text{Eq 4.3})$$

Where q_{conv} and h_c are the heat dissipation, and heat transfer coefficient, respectively. T_s is the geometry temperature, and T_∞ is the ambient temperature (293 K). The following equation represents the boundary conditions [109]:

$$K \frac{\partial T}{\partial n} + h_c (T_s - T_\infty) + \sigma\varepsilon (T_s^4 - T_\infty^4) - I = 0 \quad (\text{Eq 4.4})$$

where I is the external heat source. The conical-Gaussian model as shown in Fig 4.3 (b) is used as the moving heat source to predict the melt pool size and temperature distribution as shown in Eq 4.5 [142].

$$I(x, y, z) = \frac{6\eta P}{\pi h(r_t^2 + r_t r_b + r_b^2)} \cdot e^{[-2\frac{x^2 + z^2}{r_o^2}]} \quad (\text{Eq 4.5})$$

$$r_o(y) = r_t + \frac{y}{h} (r_t - r_b) \quad (\text{Eq 4.6})$$

where $I(x, y, z)$ is the heat intensity distribution, η is the laser absorptivity coefficient, and P is the laser power. The height, top and bottom radiuses of the heat source are defined as h , r_t , r_b , respectively. According to the literature, both the 3D Gaussian heat source with semi-spherical profile and the conical-Gaussian heat source model are commonly employed to simulate the LPBF process. Given that the melt pool formed during LPBF is often highly non-spherical, Goldak's semi-ellipsoidal power distribution is frequently adopted to more accurately capture the melt pool geometry. However, due to the inherent complexity of the Goldak model, which can pose computational challenges, the conical-Gaussian heat source serves as a practical alternative, offering a close approximation of melt pool dimensions and thermal gradients. As reported in the literature [108], the discrepancies between the conical-Gaussian and Goldak models in predicting melt pool geometry and maximum temperature are less than 5% and 10%, respectively. Furthermore, the difference in the total energy deposited into the powder layer remains below 10% between the two models. Consequently, the conical-Gaussian heat source model is deemed a suitable choice for the present simulation.

4.2.2 Structural analysis governing equations

Due to rapid melting, high-temperature phase transformations and solidification of the powders, significant thermal stress is generated within the solidified part. The presence of significant local temperature gradients gives rise to undesirable residual stresses. The corresponding static form of the mechanical equilibrium without any body force is written with Eq 4.7:

$$\nabla \cdot \sigma = 0 \quad (\text{Eq 4.7})$$

where σ denotes the Cauchy stress tensor. The total strain is divided into elastic (ϵ_e), plastic (ϵ_p), and thermal strain (ϵ_{th}) components as follows:

$$[\epsilon_{total}] = [\epsilon_e] + [\epsilon_p] + [\epsilon_{th}] \quad (\text{Eq 4.8})$$

In the present study, the elastic-perfectly plastic (EPP) model with J2 von-Mises plasticity law has been employed in the simulation to describe the plastic properties:

$$[\sigma] = [C][\epsilon_e] \quad (\text{Eq 4.9})$$

$$F_{yield} = \sigma_{vm}^{EPP} - \sigma_y \quad (\text{Eq 4.10})$$

where C is the fourth order stiffness tensor, F_{yield} is the yield function, σ_{vm}^{EPP} is the EPP von-mises stress, and σ_y is the yield strength. Interested readers are referred to [104] for further information about the coupling between thermal and mechanical field equations and boundary conditions.

4.2.3 Boundary conditions and material properties

This research used Inconel-625, a nickel-based superalloy, due to its exceptional corrosion resistance and high strength, which are highly valued in the aerospace industry. In the LPBF simulation, the initial temperature of the powder layers and substrate were set to 25 °C and 80 °C, respectively. For the thermal and mechanical analyses, the temperature-dependent material properties of the Inconel-625 were assigned to both layers and substrate [164] and the geometry of substrate was simplified. The density was set to 8440 kg/m³. The latent heat, solidus and liquidus temperatures were defined as 272 kJ/kg, 1290 °C, and 1350 °C, respectively [73]. To account for the impact of convective heat transfer within the fluid, anisotropic thermal conductivity was incorporated to achieve more accurate predictions of melt pool dimensions [119]. The top domain surface of the substrate and all exterior surfaces of the deposition were exposed to convection and radiation to the ambient environment. The convection coefficient and surface emissivity were set to 18 and 0.45, respectively [73]. The primary load on the mechanical model results from thermal stresses induced by temperature variations. Other factors such as melt pool flow, evaporation rate of solute, and material degradation after phase transformation were assumed negligible due to the objective of this study [165].

4.3 Methodology and model description

The coupled thermo-mechanical process simulation of the LPBF is a complicated multi-physics challenge, with a high level of non-linearity that needs substantial computational effort. In the following section, the MIS-based methodology is concisely explained and the simulation procedure conducted in the Abaqus software together with the developed mesoscale and macroscale models have been described.

4.3.1 Methodology

The classical IS method suggests that once the temperature of the fabricated part has cooled down, the thermal strain dissipates, and all remaining inelastic strains, aside from the plastic strain, can

be regarded as negligible. Consequently, the elastic strain is eliminated, and the plastic strain can be considered the inherent strain that remains in the part. This can be defined as follows:

$$\epsilon_{ii}^{inh} = \epsilon_{total} - \epsilon_{elastic} = \epsilon_{plastic} \quad (\text{Eq 4.11})$$

During the multi-layer modeling of the LPBF process, the shrinkage of upper layers influences the elastic properties and stress formation in the underlying depositions. As a result, the classical IS method fails to accurately predict the residual stress and distortion in this process. Therefore, in this study, the MIS method was employed to simulate the LPBF process [30]. The MIS method is an advancement of the original IS method, which was initially designed to predict residual stresses in welding applications. The MIS approach was specifically developed to differentiate between the welding and AM process simulation in using the original IS method. In the LPBF, the sequentially deposited layers act as mechanical constraints for the earlier depositions. The repeated melting and solidification cycles alter the stress and strain evolution throughout the process, continuing until the part has completely cooled to ambient temperature. For further information on the comparison between the MIS and classical IS methods in the literature, readers are referred to the previously published review article by the authors [104].

In the MIS method, inherent strains are calculated based on two key contributions: 1) compressive plastic and elastic strains at a period at when the yield strength and Young's modulus drop to their lowest levels, while the compressive plastic strain reaches its maximum point (time: t_1); and 2) the interlayer effect combined with thermal shrinkage at steady state, which occurs at room temperature (time: t_2). The anisotropic IS components can be obtained as follows:

$$\epsilon_{ii}^{inh} = \epsilon_{pii}^{t1} + \epsilon_{eii}^{t1-t2} \quad (\text{Eq 4.12})$$

where ϵ_{pii}^{t1} is the compressive plastic strain component along the three principal coordinate axes at time t_1 , ϵ_{eii}^{t1-t2} is the difference between the elastic strain component corresponding to the time t_1 and t_2 along the three principal coordinate axes. The MIS approach disregards the shear strain components of the inherent strains due to their negligible magnitudes, which have an insignificant effect on residual stress prediction [23,27].

The mesoscale model incorporates critical processing parameters in the LPBF process to provide data on melt pool size and thermal cycles, which are used to derive the MIS vectors. The

macroscale model utilizes the evaluated MIS components to compute the generated residual stresses in models similar in dimensions to the manufactured part. The following sections elaborate on the computational characteristics for each of the aforementioned model sizes.

4.3.2 Mesoscale model

The geometry and dimensions of the mesoscale model and scanning strategy are shown in Fig 4.3 (a). The computational domain is divided into two pieces including the substrate and layers. The layer thickness is 20 μm and specific number of layers are considered in the modeling for each set of process parameters to represent the melt pool and determine the thermal cycles for the t_1 period in the MIS method. The laser moves along the x direction. The element size with a higher density is assigned to the powder layers and near the interface between the substrate and powder layer. Four elements per layer is considered such a way that at least five elements were along the melt pool depth and width. To do so, the element size is set at $10 \times 10 \times 5 \mu\text{m}$ along the length, width, and depth directions, respectively. The layers are scanned with three tracks to consider the hatching space effect in the real experiments. In the thermal simulation, the elements activation is performed layer by layer and the material field variable is defined through the USDFLD subroutine code to apply the phase transformation from powder to liquid to solid states. As shown in Fig 4.3 (b), the conical-Gaussian moving heat flux parameters are calibrated using single-track experiments and then applied to the model through the DFLUX subroutine. In the mechanical simulation, the model is subjected to a thermal load derived from thermal analysis. The temperature distribution is mapped through a Python script, and the elements are activated in the vicinity of the melt pool as the laser moves. The process parameters are listed in Table 4.1.

Table 4.1 Process parameters

Parameter		Set-1	Set-2	Set-3	Set-4
Laser power (W)		200	200	200	100
Laser speed (mm/s)		1500	1000	750	1000
Hatching space (μm)		90	90	90	90
Layer thickness (μm)		20	20	20	20
Number of layers required for mesoscale modeling		5	7	11	4
Laser absorptivity coefficient		0.6	0.6	0.75	0.5
conical-Gaussian heat source dimensions	r_t (μm)	50	50	50	50
	r_b (μm)	30	30	30	30
(detailed explanation in section 4.5.1)	h (μm)	70	93	140	62

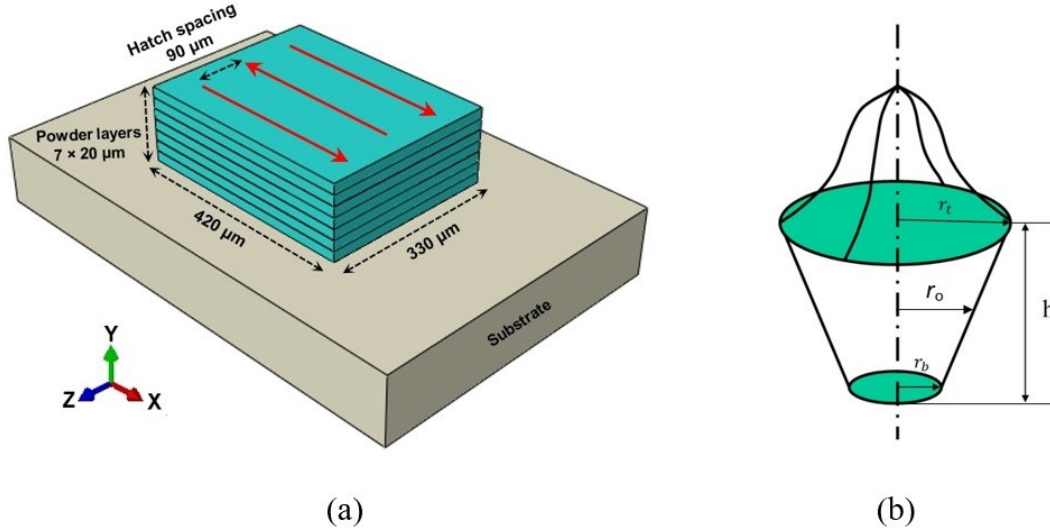


Fig 4.3 a) The substrate, build geometry and scan strategy and b) conical–Gaussian heat source model

Previous studies [133] have shown that adjusting laser scanning strategies, such as implementing zig-zag or cross-hatched patterns, can effectively reduce peak tensile stresses and tailor the mechanical properties of additively manufactured parts. Incorporating such advanced scanning strategies will be a focus of future work to further enhance model fidelity and better reflect industrial practices.

4.3.3 Macroscale model

Conventional simulation techniques are impractical for predicting residual stress and component distortion owing to their high computational expense associated with the complexity of the physical processes involved in the LPBF process. To alleviate the computational cost, the IS values calculated by the mesoscale model serve as the input to each layer for the macroscale mechanical analysis. For this purpose, the agglomeration technique is used to combine multiple physical layers into a single, larger computational layer, and the mechanical analysis is conducted. The geometry and dimensions of the macroscale part are illustrated in Fig 4.4. As shown in Fig 4.4 (b), seventy-two equivalent layers are built up as a result of merging 7 real layers. Fine element size (1 elements/layer) is considered. The IS values are introduced as the thermal expansion coefficient to each equivalent layer upon activation, and a unit temperature rise is subsequently applied. In the mechanical simulation, the material properties are defined at ambient temperature.

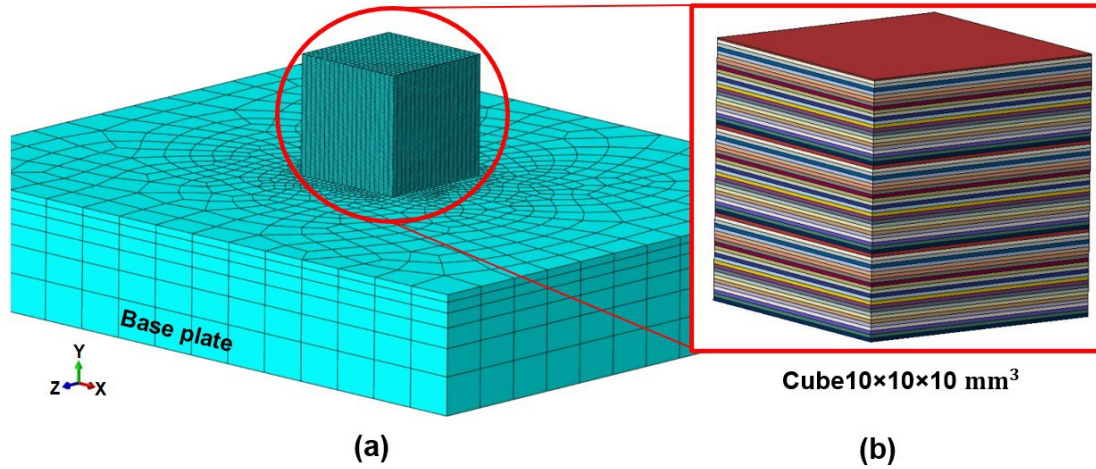


Fig 4.4 Macroscale part model; a) mesh design, and b) equivalent layers

4.4 Experimental procedures

4.4.1 Test coupon fabrication with a series of processing parameters

An EOS M290 LPBF machine was used for fabrication of Inconel-625 test coupons of 10 mm³ in the nitrogen atmosphere. The fabricated test coupons are shown in Fig 4.5. The laser is a continuous Yb (Ytterbium) fibre laser with a wavelength of 1.06 μm, which is commonly used in the LPBF process. A concentrated laser beam is adjusted via an optical system to the specified locations of the bed to fuse the particles of powder. Different processing conditions, such as scan speed and laser power, were used to experimentally characterize the variance in melt pool dimensions. Two cases of parameters were defined by considering a constant power and variable speed and then a constant speed with varying laser power. Parameter sets are provided in Table 4.2. The laser diameter and layer thickness are 100 μm, 20 μm, respectively.

Table 4.2 Processing parameters of Inconel-625 for an EOS M290 machine

Parameter case		Samples	Laser power (W)	Scan speed (mm/s)
1	Constant power	1-4	200	1500
		5-8	200	1000
		9-12	200	750
		13-16	240	1000
2	Constant speed	17-20	200	1000
		21-24	100	1000

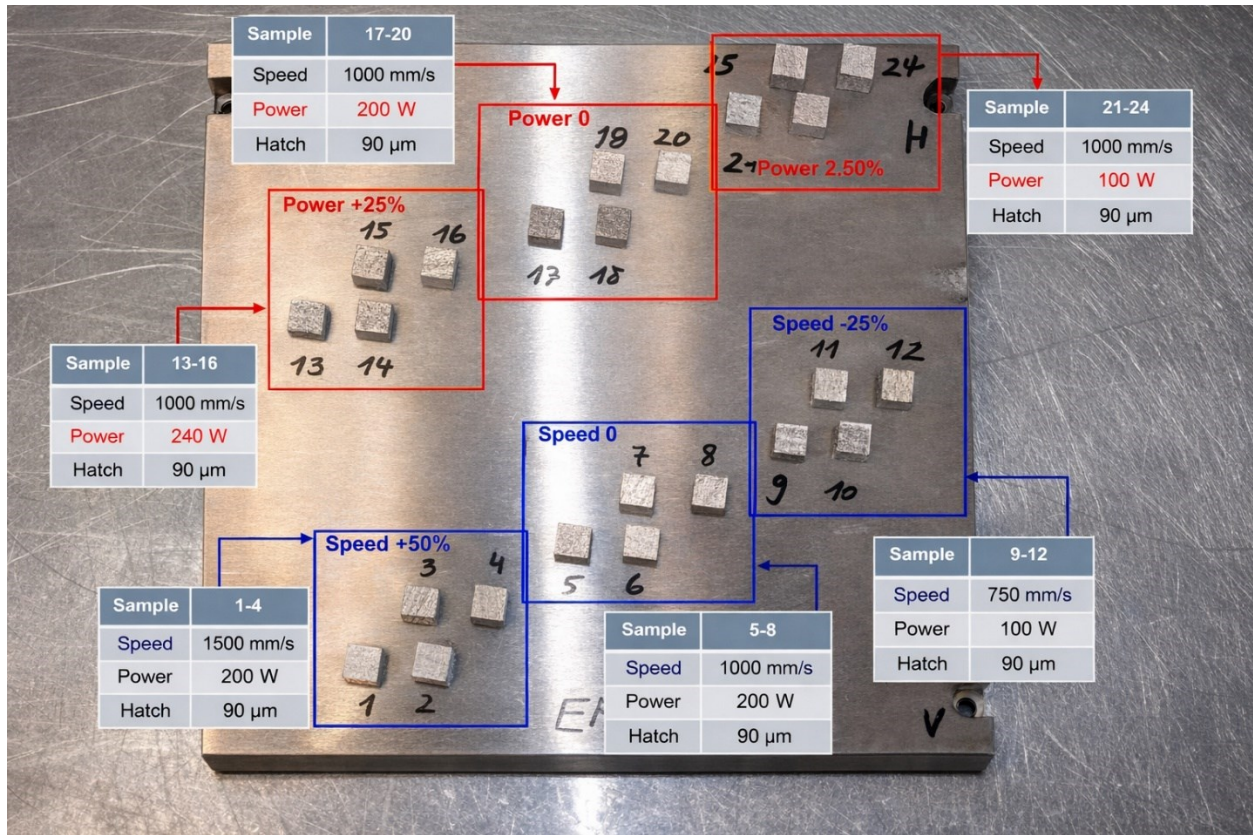


Fig 4.5 Inconel-625 test coupons manufactured by EOS M290 LPBF machine

4.4.2 Melt pool profile

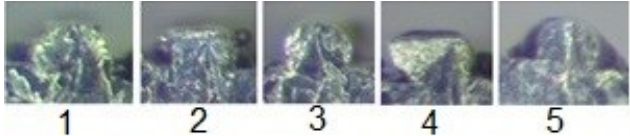
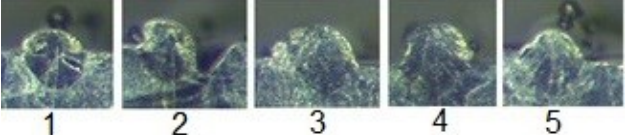
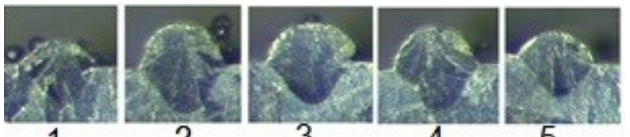
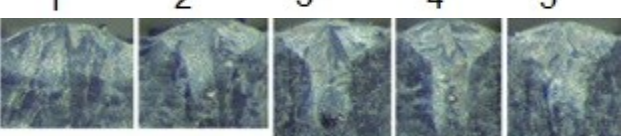
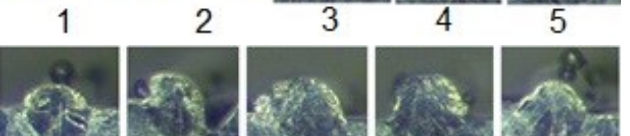
In this study, the effect of process parameters on the melt pool profile was also investigated. Multiple laser power and scan speed configurations were used to fabricate single bead specimens using EOS pre-alloyed Inconel-625 powder. The experimental process parameters are listed in Table 4.3. For each set of process parameters, 12 scans were performed, resulting in 12 beads. Fig 4.6 presents micro-section of single beads on fabricated coupons using multiple laser power and scan speed combinations after polishing and etching process



Fig 4.6 Micrographs of vertical cross-sections (Y-Z plane) of samples with 20 μ m layer thickness

To determine the geometrical characteristics of melt pool area, a scanning electron microscope (SEM) was employed. Each bead was measured at several positions (from one to twelve) to ascertain the average width and height of the melt pool. These measurements are presented in Table 4.3 for varying laser power and speed:

Table 4.3 Melt pool profiles for varying speed and power parameters

Processing condition	Melt pool profile	Melt pool size from SEM (average depth x average width)
Sample 4: Constant power (200 W) Scanning speed = 1500 (mm/s)		66 μ m x 114 μ m
Sample 8: Constant power (200 W) Scanning speed = 1000 (mm/s)		97 μ m x 127 μ m
Sample 12: Constant power (200 W) Scanning speed = 750 (mm/s)		135 μ m x 153 μ m
Sample 16: Constant speed (1000 mm/s) Power = 240 W		531 μ m x 507 μ m
Sample 19: Constant speed (1000 mm/s) Power = 200 W		115 μ m x 118 μ m
Sample 24: Constant speed (1000 mm/s) Power = 100 W		53 μ m x 68 μ m

Single beads are generated as a result of the re-melting and solidification of the plate material during a laser scan of a bare base plate [166]. The melt pool geometry was difficult to analyze for some beads created using low power (100 W). A similar issue was observed for beads created at a

high scanning speed (1500 mm/s). Single beads formed with higher power (240 W) showed significantly wider widths and greater penetration depths compared to those produced with lower power. The melt pool profiles indicate that increased laser power and/or reduced scan speed led to greater melt pool depth and width [166].

4.5 Results and discussions

Here, the numerical modeling of LPBF is divided into three main sections: the microscale heat source model, the mesoscale model (or the thermo-mechanical analysis of the powder bed to determine the IS values), and the macroscale model for the structural analysis.

4.5.1 Heat source model for microscale analysis

To achieve a reliable numerical simulation, it is necessary to first establish the parameters of the heat source model, which significantly affect the form of the molten pool and the temperature distribution [165]. A conical-Gaussian heat source is represented as a volumetric energy density, applied to the computational domain which move along the laser scanning path, considering top and bottom diameters of melt pool and penetration depth. It is noted that one of the limitations of current models is the static nature of heat source parameters, which do not account for real-time changes in the thermal field.

First, for the different process parameters, the simulated melt pool geometries did not match the actual melt pool dimensions measured by SEM, as shown in Table 4.3. Multiple iterations were conducted to confirm the agreement between the micro cross-section melt zone configuration and the heat source model generated by the simulations. Additionally, the anisotropic thermal conductivity was defined for temperatures above the melting point. Fig 4.7 illustrates the melting zone derived from the micro cross-section produced by numerical analysis. Temperatures above the melting point of the examined alloy (1320 °C) are referred to as the melt zone. It can be seen that the dimension of the melt pool size between simulations and experiments (Table 4.3) is in a reasonable agreement with an error of less than $\pm 10\%$.

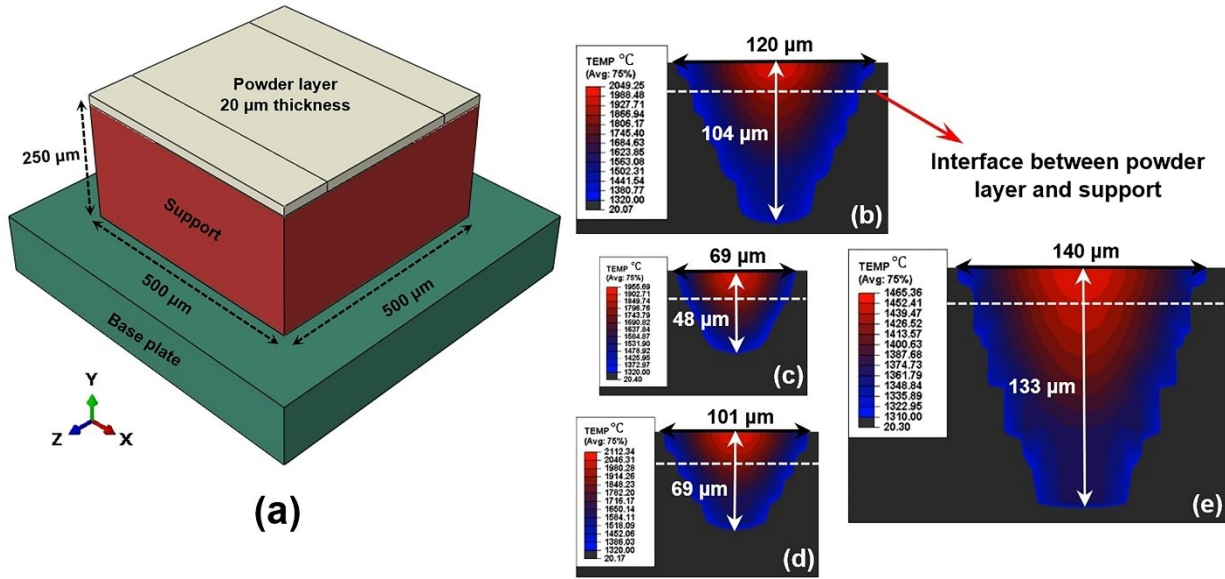


Fig 4.7 a) Simulated single track model geometry and the results of numerical melt pool dimension for b) sample 8, c) sample 24, d) sample 4, and e) sample 12 in Table 4.3

Although single-track calibration provides useful insights into melt pool dimensions, it does not fully capture the effects of multi-track interactions and overlapping thermal fields. Particularly in LPBF, where tracks overlap, the actual melt pool geometry evolves dynamically. Therefore, while the current heat source parameters offer good agreement for isolated tracks ($\pm 10\%$ error), they may require correction for full-scale parts. Future studies will incorporate multi-track and multi-layer thermal field calibration to better represent real deposition conditions.

4.5.2 Mesoscale model - thermo-mechanical analysis

In the thermal simulation, the element birth and death technique was successfully applied, where the mesoscale model analysis began with the deactivation of all elements inside the powder layers. The elements were then reactivated sequentially as each layer was deposited. This method enables the simulation of the real LPBF process with an acceptable approximation. An 8-node linear heat transfer brick element (DC3D8) in Abaqus was utilized, and a high mesh resolution was defined for powder layers. As a result of applying laser power to the powder bed, a very high-temperature gradient occurs [167]. Fig 4.8 (a, b) illustrates the scanning path in the 4th layer and a representative temperature contour after the 7th layer deposition, respectively, for parameter set-2. After sequentially scanning of all layers, the simulation of cooling down stage was characterized by a larger time step aiming to obtain the thermal equilibrium condition until 25 °C. Fig 4.9 shows the temperature history of a random element at the bottom layer. Seven and eleven temperature

peaks have been noticed as a result of the remelting process, rising to a melting point of 1320 °C for the parameter set-2 and set-3, respectively.

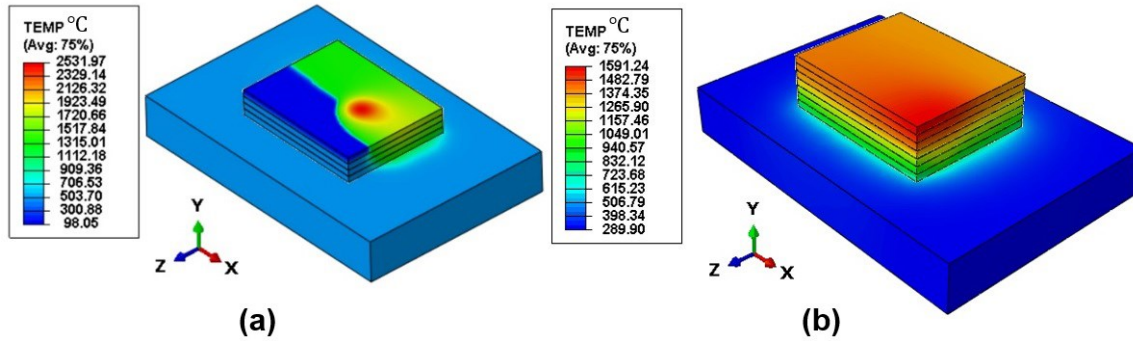


Fig 4.8 a) Temperature contour in the melt pool, and b) temperature distribution after the completion of 7th layer for parameter set-2

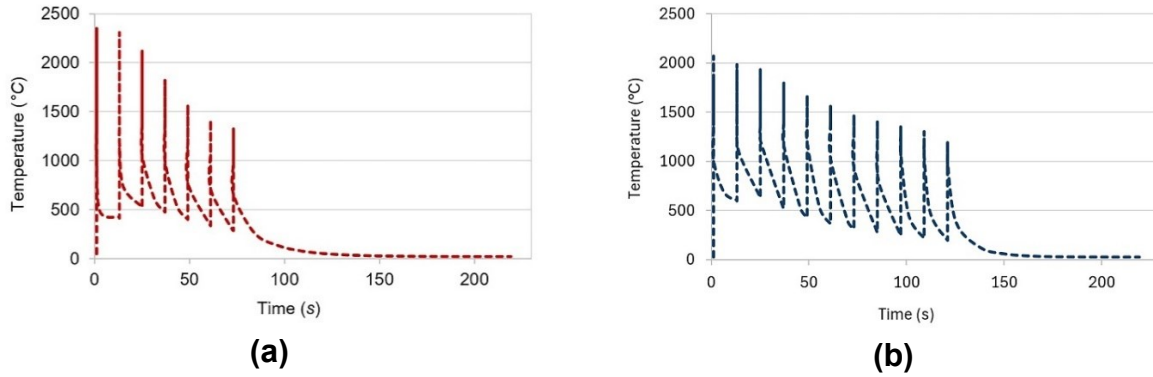
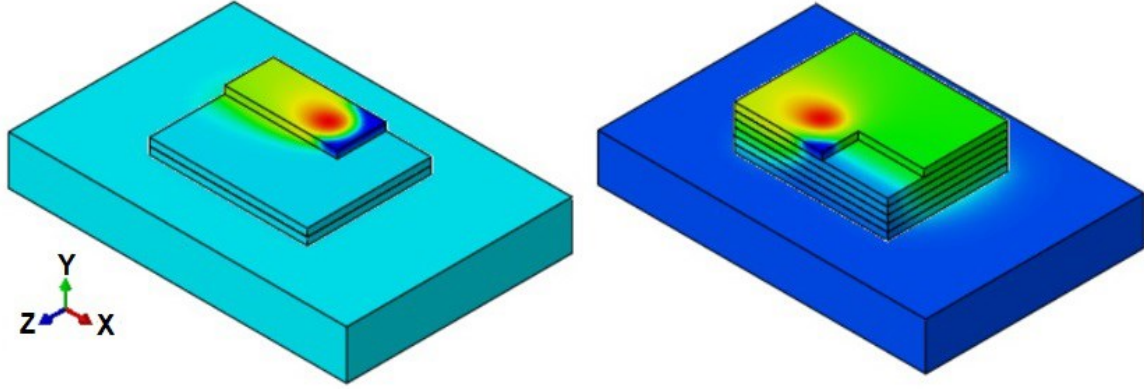


Fig 4.9 Thermal cycle at a random element in the 1st layer for a) parameter set-2 and b) parameter set-3

As explained in Section 4.3.2, the mechanical model is solely influenced by thermal stresses resulting from temperature gradients determined through the thermal simulation. The inherent strains were obtained in this analysis using the temperature histories computed at each model node. Initially, all of the elements were inactive. As the process progresses, a volume of elements is defined, and they are subsequently activated. Layer thickness, laser speed along the scanning direction, and existing time step are used to determine the volume size such that the elements therein reach a temperature higher than 10% of the melting point. The 8-node C3D8R element with reduced integration point to prevent hourglass effect was employed to construct the mechanical analysis model. Fig 4.10 illustrates the progressive element activation in the 3rd and 6th layers of the mesoscale simulation with parameter set-2. After the end of mechanical analysis was completed, the mean inherent strain vector was calculated for different parameter sets as indicated in Table 4.4.

Table 4.4 Inherent strain values for various parameter sets

Parameter	ϵ_{11}	ϵ_{22}	ϵ_{33}
Set-1	-0.0088	+0.0149	-0.0071
Set-2	-0.0139	+0.0284	-0.0166
Set-3	-0.0127	+0.0200	-0.0132
Set-4	-0.0033	+0.0062	-0.0041

**Fig 4.10** Elements activation in the 3rd and 6th layers of the simulation with parameter set-2

4.5.3 Macroscale model - structural analysis

In the macroscale model, the IS values derived from the mesoscale analysis were applied to each equivalent layer as the initial thermal strains to predict the residual stresses throughout the part. Fig 4.11 illustrates the distribution of residual stresses along the longitudinal (S_{11}), transverse (S_{33}), and build (S_{22}) directions for a cube sample simulated in the LPBF process. The analysis shows that significant residual stresses develop near the support region adjacent to the substrate. Additionally, both the longitudinal and transverse stress components exhibit their maximum values at the top surface of the cube for all parameter sets. This phenomenon in the MIS method can be attributed to four key factors. First, sequential layer-by-layer activation introduces progressive mechanical constraints, whereby newly deposited layers are increasingly restricted by the underlying, previously solidified material, resulting in cumulative stress development. Second, the purely mechanical nature of the macroscale model omits thermal effects, eliminating mechanisms such as thermal diffusion and stress relaxation that would otherwise mitigate residual stress accumulation. Third, the inherent strains are imposed instantaneously through a unit temperature rise and an artificially elevated coefficient of thermal expansion, generating abrupt stress responses without temporal moderation. Finally, the absence of stress redistribution mechanism causes the

imposed strain energy to accumulate monotonically, with the highest constraint and stress concentration manifesting in the uppermost layers.

The increased level of transverse stress (S_{33}) observed at the top surface is attributed to the transverse component of the IS vector having a greater magnitude compared to the longitudinal component. This elevated transverse stress can be linked to the effect of hatch spacing, which influences the formation of both plastic and elastic strains, as noted during the t_1 time in the mesoscale analysis.

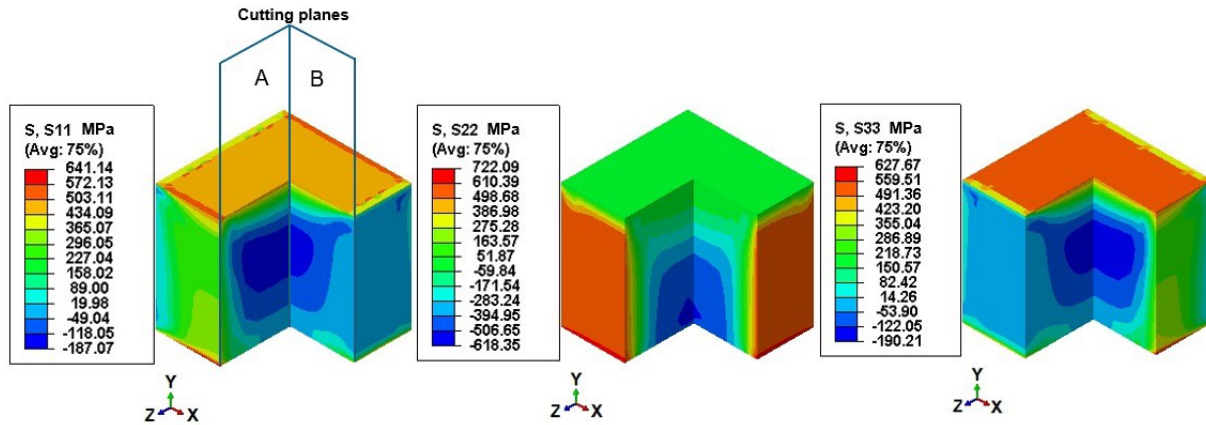


Fig 4.11 Longitudinal (S_{11}), transverse (S_{33}), and through the thickness (S_{22}) residual stresses of the cube coupon fabricated by the parameter set-2. Cutting planes, A, and B are used to show the stress distribution inside and on the sidewall of the cube

In addition to the surface-level stresses, Fig 4.12 shows how normal stress components (S_{11} , S_{22} , S_{33}) vary from the top to the bottom of the cube for different process parameter sets. The stress profiles for both S_{11} and S_{33} show a clear decreasing trend moving from the top down toward the middle of the cube, followed by a slight increase closer to the bottom. This pattern arises from the thermal shrinkage within the layer plane, which is more significant at the ends of the part compared to the center along the build direction. Prior studies have also reported similar findings using both experimental and numerical methods [30,62,122].

The S_{22} stress component, however, displays fully compressive behavior throughout the entire depth of the cube, starting at approximately zero MPa at the top surface and reaching around -600 MPa near the bottom. S_{22} approaches zero at the top layer, indicating that tensile stresses dominate at the surface while compression accumulates in the interior layers. This fully compressive trend in S_{22} reflects the anisotropic nature of stress accumulation in the LPBF process, which is

influenced by the thermal contraction during the solidification of each layer. These observations align with previous research findings [81].

The intersection of the S_{11} , S_{22} , and S_{33} curves around the midpoint (~ 3 mm) suggests a stress redistribution zone, where compressive and tensile forces begin to balance. This transition zone is likely due to the interaction between thermal gradients, material properties, and the inherent anisotropy introduced by the layer-by-layer deposition process.

Despite the insights provided by the current model, it does not fully capture the non-linear shrinkage along the build direction. This limitation stems from the MIS method's simplified thermal-mechanical coupling, which assumes constant IS values per layer and neglects the continuous evolution of shrinkage during the build process. As suggested by Liang et al. [31,86], incorporating thermal-microstructural coupling could significantly improve the accuracy of shrinkage prediction. This limitation indicates that additional thermal-microstructural coupling may be needed to more accurately represent the stress evolution throughout the build.

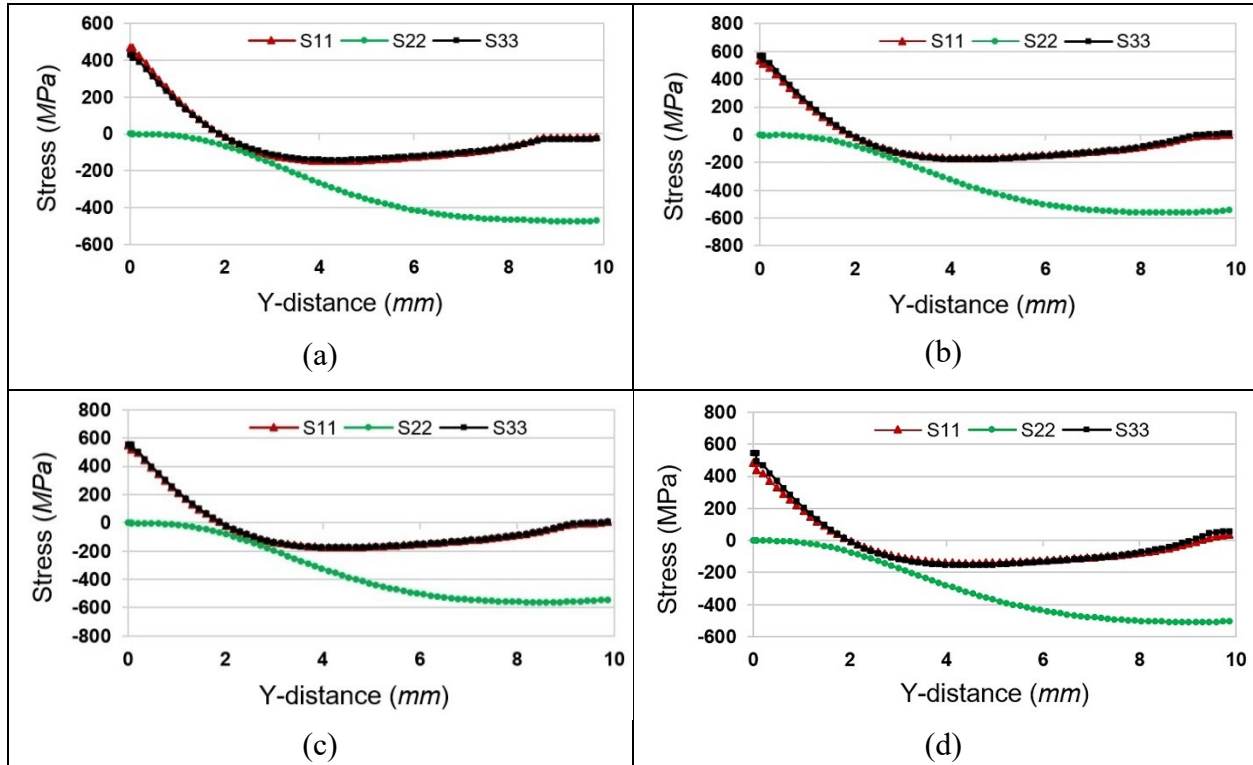


Fig 4.12 Results of the simulation showing normal stress variations along the build direction (from top to bottom) in a) sample 4, b) sample 8, c) sample 12, and d) sample 24

4.5.4 Experimental measurement of residual stresses

To validate the accuracy of the FE analysis, residual stresses were experimentally measured using the X-ray diffraction (XRD) method, as depicted in Fig 4.13. The residual stress analysis was performed on the surface of the fabricated LPBF coupons ($10 \times 10 \times 10 \text{ mm}^3$) and at depths of 1000 μm , 2000 μm , and 3000 μm using a G3 X3000 diffractometer from Stresstech at the advanced facilities of Siemens, Germany.



Fig 4.13 Residual stress measurement using the G3 X3000 diffractometer from Stresstech

Due to the limited penetration ability of soft X-rays in metals, analyzing residual stresses at greater depths requires material removal. Traditional material removal techniques, such as machining or milling, often introduce mechanical forces that can lead to the introduction of new stresses, thereby skewing the residual stress measurement results. To address this, electrochemical etching is typically employed as it minimizes the risk of additional mechanical stresses. Despite its benefits, electrochemical etching has certain limitations, including a relatively slow rate of material removal, particularly when targeting significant depths. Additionally, it may produce uneven surfaces at greater depths, which could affect the accuracy of residual stress measurements, especially in small areas or for layers up to 3000 μm in depth.

To overcome these challenges, a hybrid approach combining mechanical milling and electrochemical etching was used. This method was selected to balance the efficiency of bulk material removal with the precision of electrochemical etching, ensuring minimal stress

introduction. Pre-tests confirmed that milling-induced stresses were negligible beyond a 200 μm depth, validated by consistent XRD measurements after electrochemical etching, as shown in Fig 4.14. This hybrid approach leverages the speed and efficiency of mechanical milling for bulk material removal, followed by electrochemical etching to ensure an almost flat surface without the introduction of residual stresses from the milling process, addressing concerns about milling-induced stresses noted in prior studies [62].

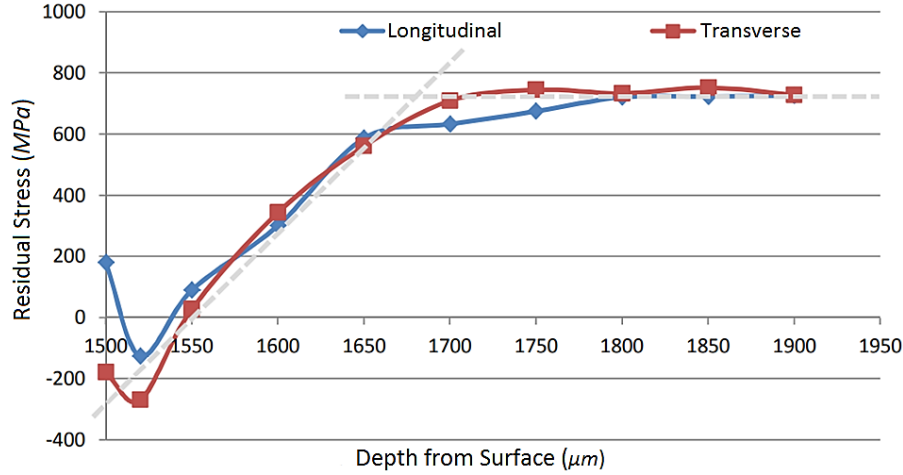


Fig 4.14 Residual stress profile of sample #20 after mechanical milling of 1500 μm

In Fig 4.14, the residual stress graph reveals a significant reduction near the surface after milling (around 1500 μm in depth). Both longitudinal and transverse stresses increase with depth, eventually stabilizing after about 1750 μm , where the effects of milling subside. The gray auxiliary lines in the figure indicate that residual stresses are impacted by the machining process up to a depth of about 200 μm from the milled surface. To ensure accuracy in the stress analysis and to account for any stress introduced by machining, a safety margin of 100 μm was added. In this test series, material was removed mechanically except for the final 300 μm , which was etched electrochemically to eliminate any residual stresses that might have been introduced during milling.

Mechanical milling, while effective for material removal, can inadvertently induce partial stress relaxation during the process, potentially altering the original residual stress state prior to measurement [168]. This alteration arises from the redistribution of stresses as material is removed, leading to potential inaccuracies in subsequent analyses. Additionally, the milling process often results in increased surface roughness and subsurface damage, which can influence the strain

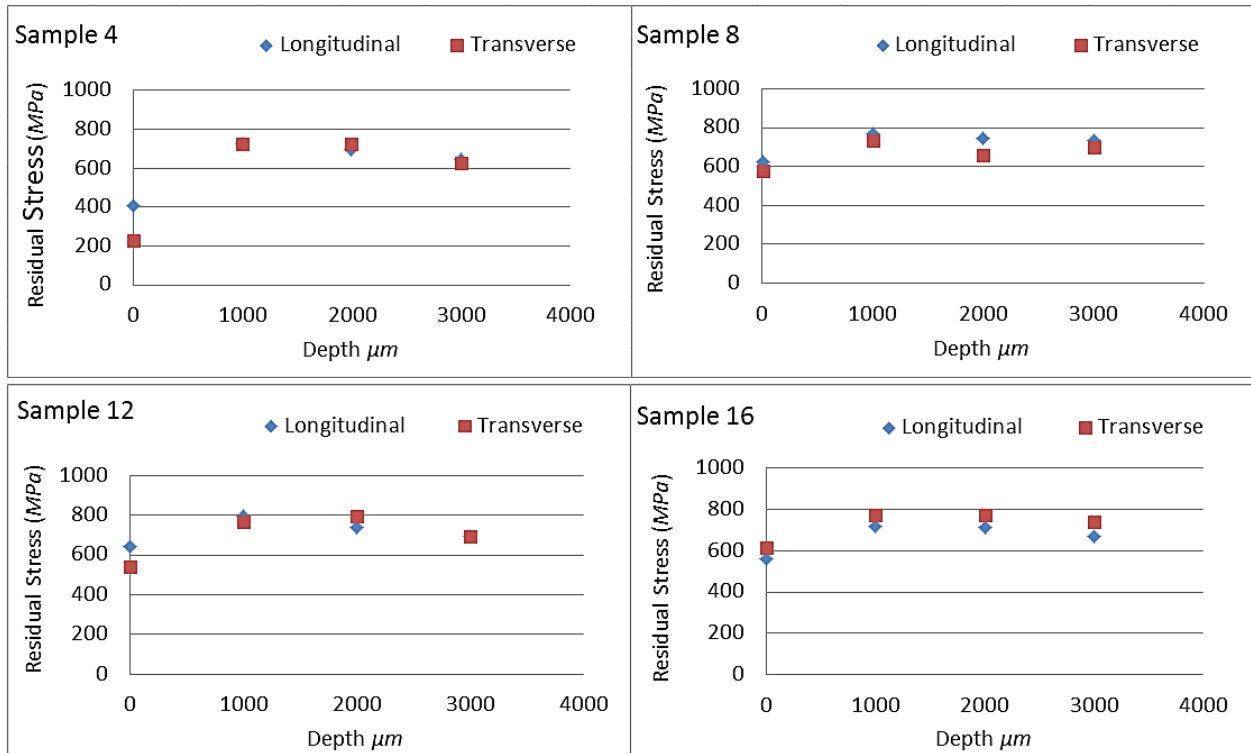
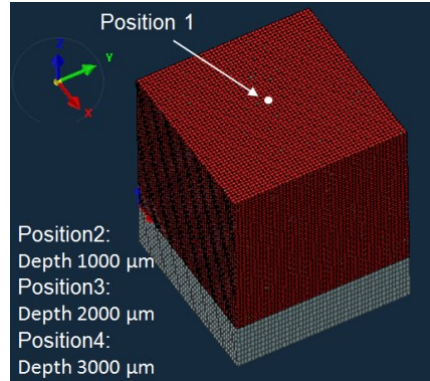
release behavior during electrochemical etching, thereby affecting the accuracy of residual stress measurements. Precise depth control during both milling and etching is crucial; any deviations can introduce uncertainties into the residual stress depth profile, compromising the reliability of the data. While the hybrid milling–electrochemical etching technique has significantly advanced subsurface residual stress characterization, these challenges highlight the need for further refinement of the methodology to enhance measurement accuracy and reliability.

To address these limitations, ion milling, particularly when implemented through Focused Ion Beam (FIB) techniques offers several advantages that can enhance the reliability of residual stress assessments [169]. FIB milling enables the creation of features with sub-micron precision, facilitating detailed stress analysis in microstructures and thin films. Unlike mechanical methods, ion milling is a non-contact technique that reduces the introduction of artifacts such as scratches or smearing, preserving the integrity of the sample. When combined with Digital Image Correlation (DIC), FIB milling allows for precise measurement of displacement fields resulting from stress relaxation, leading to accurate residual stress quantification. Incremental ion milling facilitates the assessment of residual stress variations with depth, providing a comprehensive understanding of stress distributions within the material.

Residual stress analysis by X-ray diffraction stress analysis was performed by a G3 X3000 diffractometer provided by Stresstech. Using Mn-KD radiation, the 311-reflection of Inconel-625 was analyzed by position-sensitive detectors. The X-ray spot on the sample was limited by a collimator with a diameter of 3 mm in diameter. After linear background correction, the diffraction profiles were evaluated by cross-correlation algorithms. Residual stresses were determined according to the classical $\sin^2\psi$ -method applying 11 ψ -angles in the range of $\pm 45^\circ$, a method validated for LPBF applications in prior studies [59]. As specific X-ray elastic constants (XECs) for LPBF Inconel-625 were not available, they were calculated according to the Voigt's model assuming a Young's modulus of 208 GPa and a Poisson's ratio of 0.28. Voigt's model here refers to elastic averaging of polycrystalline grains assuming uniform grain used to estimate X-ray elastic constants from bulk Young's modulus and Poisson's ratio. According to the Voigt elastic averaging assumptions, polycrystal is elastically uniform, grains are perfectly bonded, and no stress concentration is at grain boundaries [170]. Although calculated stresses are directly dependent on

the XECs, they only affect the absolute stress values, not the relative comparison between calculated stresses.

The results, which summarize residual stresses for all six cubes (illustrated in Fig 4.5), considering different laser power and scanning speed conditions, are illustrated in Fig 4.15. The longitudinal stress refers to residual stress in the x-direction, parallel to the laser scanning direction, while the transverse stress refers to residual stress in the y-direction, perpendicular to the scanning direction.



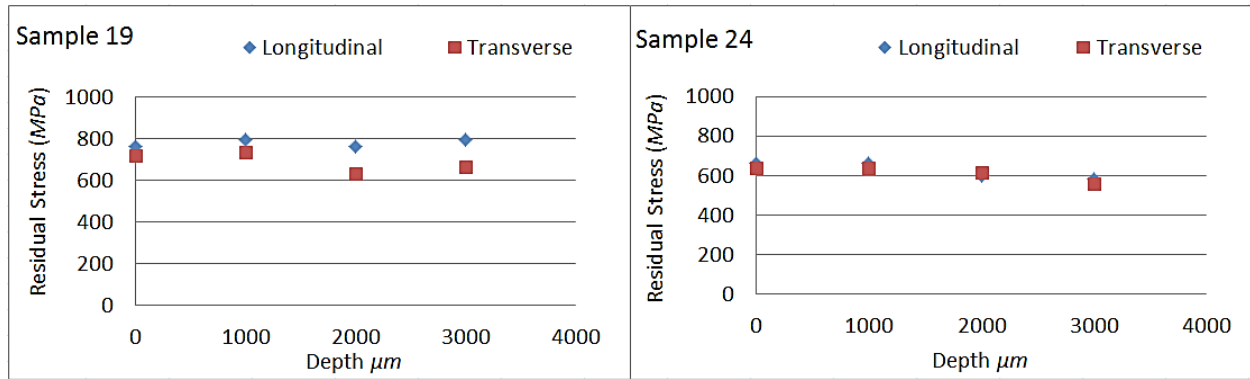


Fig 4.15 Longitudinal and transverse stresses in six coupons

Samples 4, 8, and 12 were fabricated with a constant laser power of 200 W and varying scanning speeds: 1500 mm/s (Sample 4), 1000 mm/s (Sample 8), and 750 mm/s (Sample 12). The results indicate that residual stress increases as scanning speed decreases. As shown in Fig. 15, Sample 12 exhibits the highest surface longitudinal stress at ~640 MPa and transverse stress at 540 MPa, while Sample 4 shows the lowest at ~406 MPa (longitudinal) and ~230 MPa (transverse). This trend extends beneath the surface, where slower scanning speeds correspond to higher residual stresses throughout depth. However, the stress magnitudes do not consistently decrease with depth. In fact, both stress components often increase from the surface to 1000 μm, sample 12's longitudinal stress rises to ~800 MPa, before gradually reducing at greater depths.

Samples 16, 19, and 24 were produced at a fixed scanning speed of 1000 mm/s with varying laser powers: 240 W (Sample 16, SEM images reveal an unusually large and deep melt pool (approximately 531 μm × 507 μm), characteristic of keyhole formation), 200 W (Sample 19), and 100 W (Sample 24). Higher laser power results in increased residual stress. As shown in Fig. 15, Sample 16 exhibits surface stresses (longitudinal: ~560 MPa, transverse: ~615 MPa), followed by Sample 19 (longitudinal: ~795 MPa, transverse: ~765 MPa) and Sample 24 (longitudinal: ~665 MPa, transverse: ~640 MPa). Excluding Sample 16 due to keyhole mode effects, Sample 19 (200 W) shows higher surface stresses than Sample 24 (100 W), confirming the trend. This pattern persists at 1000 μm depth, where stresses peak, Sample 19's longitudinal stress reaches ~800 MPa, and Sample 24's reaches ~670 MPa, before decreasing at greater depths, consistent with the observed depth profile behavior. These results suggest that, within the studied range, variations in laser power have a somewhat more pronounced influence on the magnitude of residual stresses than changes in scanning speed, aligning with trends reported in prior studies [126,133,171,172].

Fig 4.16 compares the residual stress profiles at the surface and at depths of 1000 μm , 2000 μm , and 3000 μm for different laser power settings.

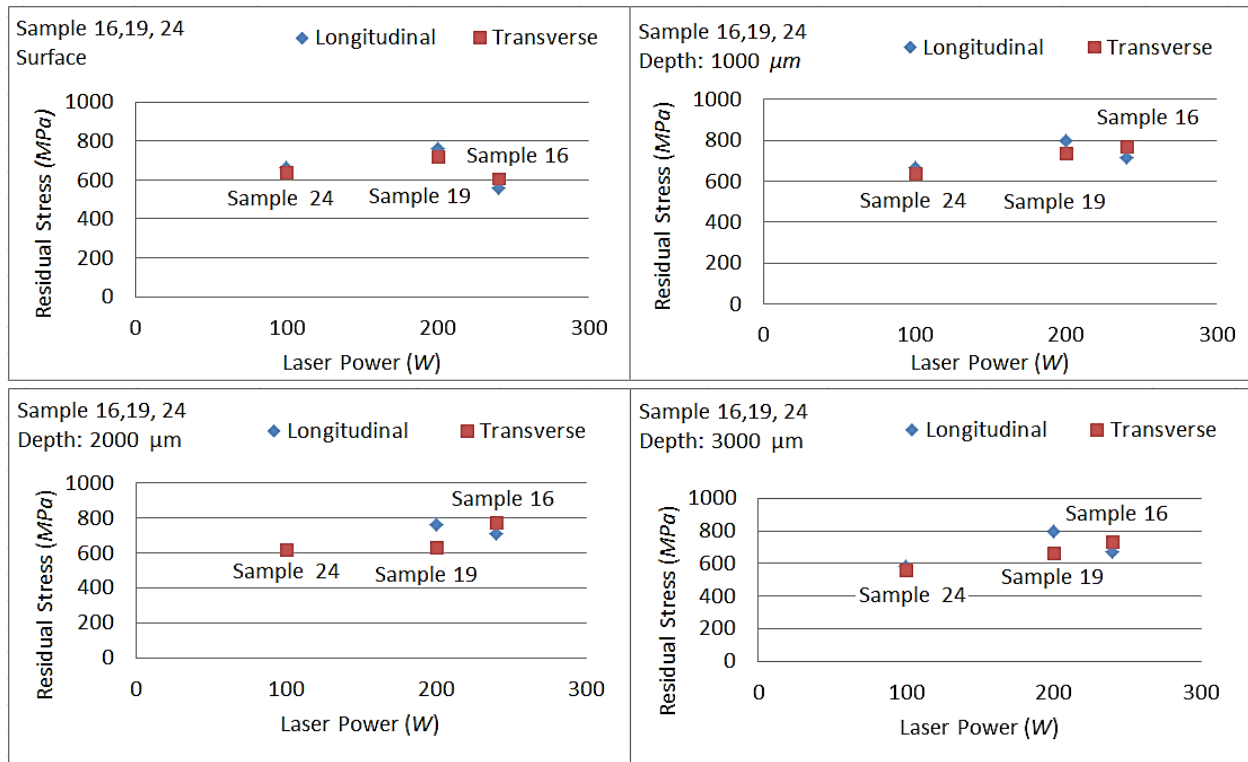


Fig 4.16 Variation of longitudinal stress and transverse stress at surface, 1000 μm , 2000 μm , and 3000 μm depth due to variations in the laser power

Increasing the laser power leads to higher maximum melt pool temperatures, which, in turn, intensify thermal gradients during solidification and ultimately lead to larger residual stresses [171]. As shown in Fig 4.16, this trend is generally evident in Samples 24, 19, and 16, fabricated at powers of 100 W, 200 W, and 240 W, respectively. However, it is important to differentiate between conduction mode (Samples 24 and 19) and keyhole mode melting (Sample 16). At the surface, Sample 19 (200 W, conduction mode) displays the highest residual stresses among the conduction mode samples (longitudinal: ~795 MPa, transverse: ~765 MPa), followed by Sample 24 (100 W, longitudinal: ~665 MPa, transverse: ~640 MPa). These findings are consistent with previous studies (Ref. [172]), that predicted increased residual stresses at higher laser power levels due to more pronounced thermal effects. Interestingly, Sample 16 (240 W), although processed at a higher power, shows slightly lower surface stresses (longitudinal: ~560 MPa, transverse: ~615 MPa). This anomaly can be attributed to the transition into keyhole mode at 240 W, where unstable melt pool dynamics and vapor-induced cavity formation led to complex heat flow and stress

redistribution. This finding highlights the importance of avoiding keyhole mode in LPBF for applications requiring predictable stress profiles, as the isotropic heat flow and stress redistribution can compromise part quality. Future studies could explore optimized process parameters to maintain conduction mode while maximizing energy input.

At a depth of 1000 μm , the increasing trend in stress magnitude with laser power continues, with all three samples exhibiting peak stresses at this depth. However, while Samples 24 and 19 maintain the expected pattern of longitudinal stresses being higher than transverse ones, Sample 16 begins to deviate. At greater depths (2000 μm and 3000 μm), the transverse residual stress in Sample 16 becomes comparable to, or even exceeds, the longitudinal stress, a pattern not observed in the conduction mode samples. This shift is indicative of the distinct thermal and mechanical behavior induced by keyhole mode processing. The deep and narrow melt pool geometry under keyhole conditions promotes radial and more isotropic heat flow, reducing the directional bias typically seen in conduction mode. Consequently, residual stress arising from thermal contraction are more evenly distributed, reducing the dominance of longitudinal stress and increasing transverse stress magnitudes. These results underscore two key observations: (1) increasing laser power under conduction mode amplifies residual stress magnitudes due to steeper thermal gradients, and (2) transitioning to keyhole mode not only increases the overall stress level but also modifies the stress orientation, with a noticeable rise in transverse stress relative to longitudinal stress. This underscores the necessity of distinguishing between conduction and keyhole melting regimes when assessing how process parameters influence residual stress development in LPBF processes.

Fig 4.17, compares the longitudinal and transverse stress profiles for different scanning speeds. As scanning speed decreases, residual stresses increase throughout the depth of the build due to greater heat input and more pronounced thermal gradients. Samples 4, 8, and 12, all produced at a constant laser power of 200 W but at scanning speeds of 1500 mm/s, 1000 mm/s, and 750 mm/s respectively, exhibit a consistent trend across all depths. At the surface, Sample 12 (slowest scan speed) shows the highest longitudinal and transverse stresses (~ 640 MPa and ~ 540 MPa), while Sample 4 (fastest scan speed) shows the lowest (~ 406 MPa and ~ 230 MPa). This pattern persists at 1000 μm and 2000 μm , where the stresses continue to rise with decreasing scan speed—reaching

peak longitudinal values of ~ 795 MPa for Sample 12 and only ~ 700 MPa for Sample 4 at $2000 \mu\text{m}$.

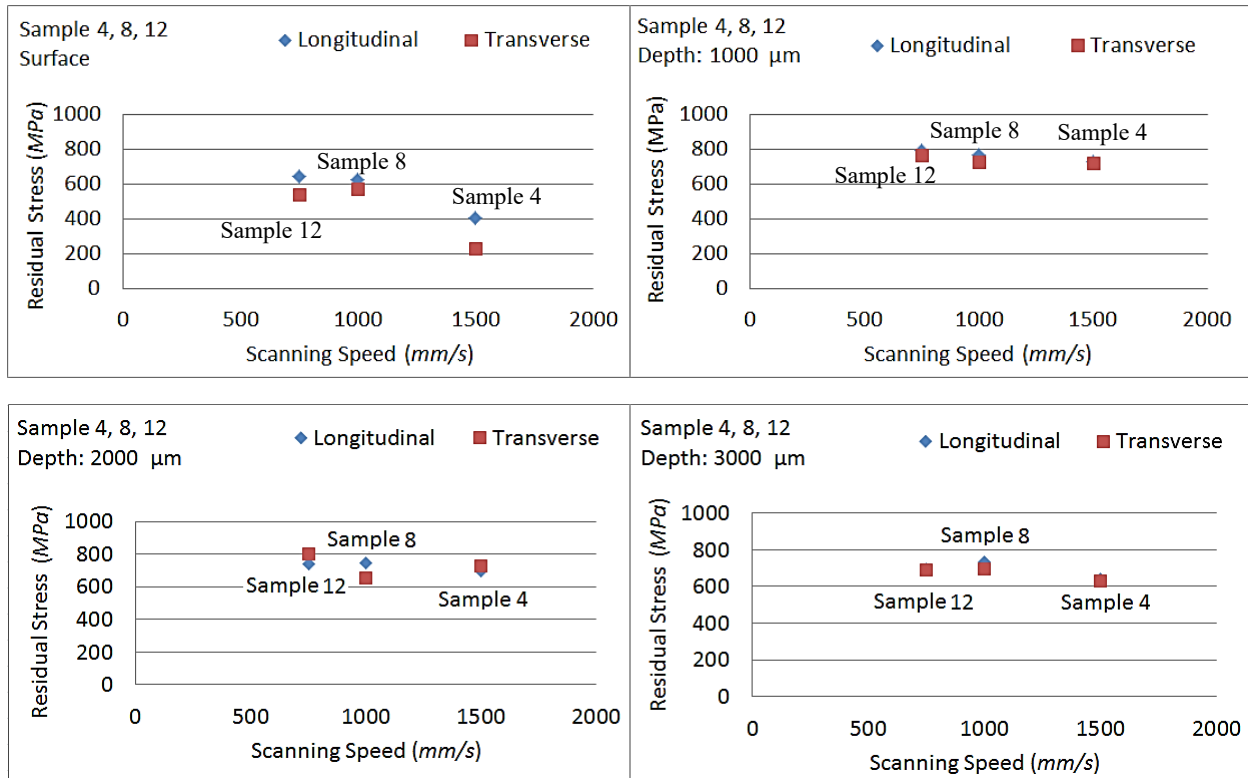


Fig 4.17 Variation of longitudinal and transverse stresses at surface, $1000 \mu\text{m}$, $2000 \mu\text{m}$, and $3000 \mu\text{m}$ depth due to variations in the scanning speed

Depth-dependent analysis reveals that the residual stresses do not monotonically decay with depth. Instead, for all samples, stresses tend to increase from the surface to $1000 \mu\text{m}$ or $2000 \mu\text{m}$ before slightly declining at $3000 \mu\text{m}$. This non-linear profile suggests that peak stress accumulation occurs subsurface, likely due to thermal gradients being most severe in that region during solidification. Notably, at $3000 \mu\text{m}$, Sample 12 still maintains the highest residual stress values (~ 700 MPa), indicating the lasting influence of lower scan speed deep into the part. Moreover, longitudinal stress consistently exceeds transverse stress at almost all depths, underscoring a directional bias in stress development that is more resilient to depth changes under slower scanning conditions.

These observations confirm that scanning speed influences not only the magnitude but also the depth-wise distribution of residual stresses. However, the degree of anisotropy and the overall stress levels induced by scanning speed variations are still less dramatic compared to changes driven by laser power. Thus, while scanning speed plays a meaningful role in shaping the residual

stress profile through the build thickness, laser power remains the more dominant factor in both surface and depth-resolved stress evolution in LPBF processes.

4.5.5 Comparison of experimental and simulation data

Experimental residual stress measurements obtained using XRD were also used to thoroughly validate the predicted residual stresses from the simulation. The comparison was made at the center of the surface and at three depths: 1000 μm , 2000 μm , and 3000 μm . Fig 4.18 illustrates the predicted versus measured longitudinal and transverse residual stresses across the entire deposition process for various parameter sets. The parameter sets 1–4 correspond to Samples 4 (200 W, 1500 mm/s), 8 (200 W, 1000 mm/s), 12 (200 W, 750 mm/s), and 24 (100 W, 1000 mm/s), respectively, covering a range of scanning speeds and laser powers.

For both the longitudinal and transverse stresses, the predicted residual stresses closely align with XRD measurements at the surface (0 mm depth). Specifically, the longitudinal stress shows a reasonable degree of correlation, with the predicted stress with an error of less than 14 % for the parameter sets 1, 2, and 3. On the other hand, the transverse stress is almost identical for the parameter sets 2,3, and 4 with an error of 1 %, 0.8 %, and 12 %, respectively, indicating high accuracy for most sets, though set 4 shows a slightly larger discrepancy.

When examining the depth dependence, significant discrepancies emerge. In the numerical simulation, the tensile residual stress decreases rapidly with increasing depth, a pattern consistent with prior studies using the MIS approach [30,90,122]. In contrast, experimental XRD reveal that the maximum tensile residual stress occurs just below the top surface, at approximately 1000 μm depth, and decreases only marginally as the depth increases. It can be seen from the plot that the general trend between simulation and experiment is inconsistent. The error can be attributed to the inherent limitations of the MIS-based FE model used for the subsurface stress predictions. This model simplifies the thermal-mechanical coupling involved in layer-by-layer AM processes, particularly in predicting how thermal gradients and mechanical stresses interact below the surface, as noted in prior studies [161]. While the model successfully predicts stress near the surface, where thermal gradients are most pronounced, it tends to underestimate the stress in the deeper layers. Consequently, the numerical simulation exhibits a rapid decrease in tensile stress with depth, while experimentally, the stresses remain relatively high just beneath the surface and decrease more gradually. To mitigate this limitation, future refinements could incorporate non-uniform strain

distributions by integrating adaptive strain calibration based on layer-specific thermal histories, potentially improving the accuracy of subsurface stress predictions.

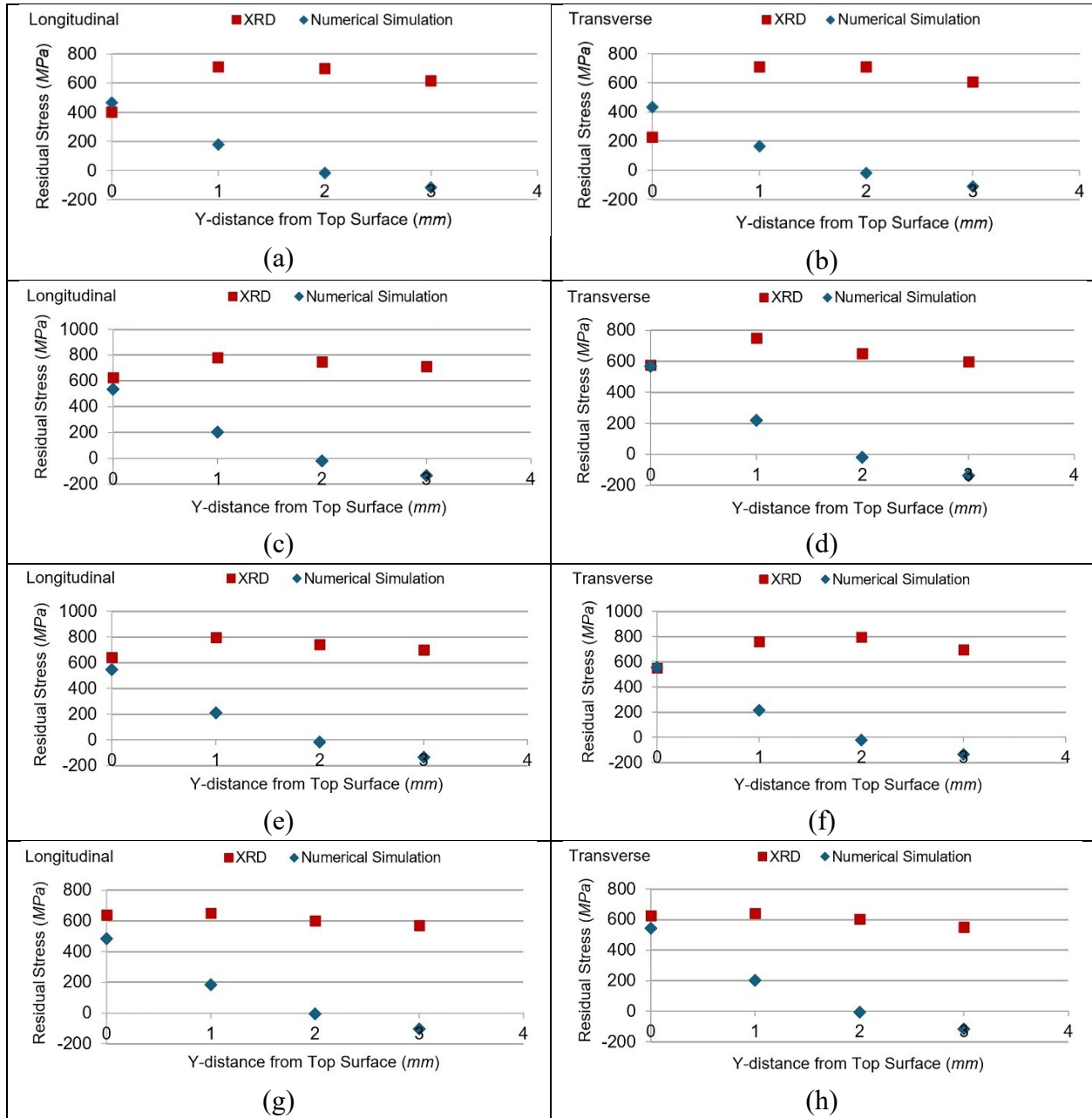


Fig 4.18 The comparison of the predicted and measured longitudinal and transverse stresses at 1000 μm , 2000 μm and 3000 μm depth from surface for a, b) parameter set-1; c, d) parameter set-2; e, f) parameter set-3 and g, h) parameter set-4

One explanation for this discrepancy is the assumption of uniform plastic strain in the MIS model, which does not fully account for the non-homogeneous nature of stress accumulation deeper within the part. In the LPBF process, the topmost layer, being the last to solidify, cools without further

reheating and is thus less constrained, allowing partial stress relaxation. In contrast, the subsurface layers experience multiple thermal cycles from the deposition of subsequent layers, leading to repeated thermal expansion and contraction without sufficient opportunity for plastic relaxation. These layers are mechanically constrained by both the previously solidified material below and the newly deposited layers above, amplifying the development of tensile stress. Additionally, the constraint gradient through the depth of the part results in increased mechanical resistance to deformation for the subsurface layers. Finally, differences in cooling rates, wherein subsurface regions cool more slowly due to heat accumulation and insulation from surrounding material, promote steeper thermal gradients and higher plastic strain, further contributing to the elevated tensile residual stresses beneath the top surface. The experimental results suggest that the maximum residual stress occurs below the surface, around 1000 μm in depth, a feature the MIS model fails to capture accurately.

In this study, a cube as a simple geometry was chosen to investigate the residual stress variation. As a result, the MIS method underestimates the residual stress prediction compared with experiments along the build direction. On the other hand, since the MIS method has proven its fidelity to predict residual distortion and residual stress on the top layer, other numerical approaches like equivalent heat source method can be employed for residual stress prediction along the build direction. This approach is based on the part activation model, which accounts for the heating and cooling processes. The mechanical characteristics of the equivalent powder layer are different under the corresponding heating and cooling conditions [161,173]. Therefore, the mechanical performance predicted by the equivalent heat source method can be more accurate.

4.6 Summary and conclusions

A multi-scale MIS-based FE modeling approach has been developed for efficient prediction of residual stress in part produced by the LPBF process. The melt pool dimensions for the benchmark samples have been carefully measured, and the obtained results have been subsequently used as an input to determine the heat source model. Incorporating adaptive, real-time heat source models could significantly improve the fidelity of residual stress predictions, particularly for complex geometries. In the microscale simulation, a Gaussian heat source distribution with adjusted dimensions has been applied based on cross-sections acquired from the SEM.

The FE model developed for the heat source and the mesoscale model consider as inputs the most important processing parameters required for the LPBF manufacturing of parts such as laser power, laser speed and exposure time. The temperature profile developed by the thermal model has been then utilized as an input for the mesoscale mechanical simulation. The obtained IS values from the mesoscale model were fed into the macroscale model to predict the residual stresses. The developed model was then compared with experimental results for residual stresses conducted using XRD on the selected coupons. Additionally, the effects of LPBF process parameters including the beam power and speed on residual stresses were investigated.

Although the model demonstrated reasonable accuracy at the surface, discrepancies at greater depths suggest that the MIS method, while computationally efficient, might need refinement for predicting stresses in multi-layer builds. In conclusion:

- The MIS-based FE model predicts surface residual stress in LPBF parts with errors less than 14% for longitudinal stress and up to 12% for transverse stress, validated against XRD measurements on Inconel-625 coupons. This finding is supported by the study's validation data, showing high accuracy for near-surface predictions.
- The MIS-based FE model significantly underestimates tensile residual stresses beyond 1 mm in depth, where experimental XRD data show a stress peak around this depth, contrary to the model's prediction of a rapid decline. This mismatch reveals the model's limitations in accurately capturing subsurface stress evolution. These limitations stem from the inherent assumptions of the MIS method, such as uniform plastic strain and simplified thermal-mechanical coupling, which constrain its predictive capability—particularly in multi-layer LPBF builds. The model's inability to account for transient thermal effects further contributes to its inaccuracy in deeper layers, underscoring the need for more advanced modeling approaches to improve subsurface stress prediction.
- Laser power significantly influences residual stress, with an increase of approximately 20% in longitudinal stress from 100 W to 200 W at constant scanning speed (1000 mm/s). However, at 240 W (keyhole mode), the stress decreases to levels lower than at 200 W (~560 MPa vs. ~795 MPa), indicating a non-monotonic trend. Scanning speed also affects residual stress, with higher speeds (1500 mm/s) resulting in lower stresses (~406 MPa) compared to lower speeds (750 mm/s, ~640 MPa) at constant laser power (200 W).

- The hybrid milling-electrochemical etching method used for sample preparation may introduce surface artifacts, potentially affecting the accuracy of XRD measurements at deeper layers. This limitation was identified in the study's experimental methodology, suggesting a need for improved techniques like ion milling.

Chapter 5 An advanced finite element–AI coupled framework for high-fidelity and efficient prediction of residual stresses and distortions in laser powder bed fusion

Abstract: This research introduces a methodology to estimate inherent strains (IS) in Laser Powder Bed Fusion (LPBF) process by combining a high-fidelity, experimentally-validated finite element (FE) model with machine learning (ML) techniques. The main objective is to enhance computational efficiency in the non-linear coupled thermo-mechanical simulations and thus accelerate the prediction of residual stresses and consequently distortions for part-scale components. The FE model leverages the modified IS approach at the mesoscale. Five ML models are effectively used to efficiently predict simulation data. A comprehensive set of key independent variables was identified and used to train the ML models, including key LPBF processing parameters (laser power, scan speed, layer thickness, hatching space, and scanning strategy), build-height nodal coordinate and nodal temperatures extracted from FE thermal simulations. To enhance the applicability of the developed surrogate ML models, three commonly used nickel-based superalloys were selected to enable generalization across different material types. Among all the developed ML models, categorical boosting (CatBoost), k-nearest neighbors (KNN), and optimized KNN exhibited the highest predictive performance for inherent strains in the longitudinal, transverse, and layer-thickness directions, with respective relative errors of 16.5%, 16.3%, and 22.5% compared to FE results. The proposed ML–FE approach accelerates computation by up to 10,000× compared to traditional FE methods while maintaining distortion prediction errors below 16% for cantilever beam geometries. This framework highlights how data-driven modeling can significantly enhance the efficiency and scalability of physics-based simulations in metal additive manufacturing, paving the way for rapid process parameter optimization.

5.1 Introduction

Laser Powder Bed Fusion (LPBF) is a layer-wise metal additive manufacturing (AM) technique in which successive micron-thick layers of powder are melted by a high-power laser within an inert environment to build complex geometry components. The CAD model of the part is sliced

into thin layers; a re-coater evenly spreads powder, which the laser selectively fuses, and the platform lowers to repeat the cycle until the part is complete. LPBF offers unparalleled design flexibility, enabling high-precision internal features, reduced material waste, and near-net-shape fabrication, while producing refined microstructures that often enhance mechanical performance [174–177]. Despite these benefits, a major challenge limiting broader adoption is the formation of detrimental residual stresses. These stresses arise from steep thermal gradients and rapid solidification, leading to accumulated tensile stresses that cause part distortion, warping, delamination, and cracking, particularly during cooling or after removal from the build plate [178,179]. Recent investigations have shown that scanning patterns, energy density, and build-plate preheating can significantly affect stress accumulation [128,180–184].

Over the last decade, numerical and data-driven approaches have become promising alternatives to extensive experimental campaigns for predicting induced residual stresses and distortions in LPBF process. High-fidelity thermo-mechanical simulations provide detailed insights into temperature gradients, phase transformations, and stress evolution during the build process. The LPBF process simulation is mainly based on the detailed thermo-mechanical approach, either fully coupled or partially (sequentially) coupled methods [104]. The computational burden of these simulations arises from the need to resolve rapid thermal fluctuations through fine temporal discretization, use high-resolution meshes to capture steep temperature gradients near the melt pool, and concurrently address coupled thermal and mechanical fields [8,57,58,60]. Despite the development of various simplification techniques, such as layer lumping [63], adaptive mesh refinement [66], multi-scale modeling [37], and reduced-order heat transfer approaches [20], the simulation of complex industrial LPBF parts remains computationally intensive, with limited improvements in overall efficiency. Recently, the inherent strain (IS) method and its modified variants have demonstrated their effectiveness in predicting generated residual stresses and distortions in the LPBF process [21,30,136]. Nevertheless, the predictive capability of this otherwise robust methodology is limited by key challenges, most notably the accurate characterization of non-uniform strain distributions. This limitation stems from the need for adaptive calibration procedures that account for the layer-specific thermal histories inherent to the process [183]. Additionally, the method is sensitive to geometric variations, further increasing the computational cost for the calculation of inherent strains in complex part geometries [185].

To address this challenge, limited recent studies have leveraged advanced artificial intelligence (AI) techniques, by integrating machine learning (ML) with the finite element (FE) methods in metal AM, for applications including defect detection (residual stresses and distortions), process parameter optimization, prediction of inherent strain, fatigue life, and part distortion compensation [186–188]. For example, Mohajernia et al. [189] developed a novel framework to investigate the geometrical and mechanical properties of single bead clads in the directed energy deposition process. Empirical data were employed to calibrate FE models, with both datasets serving as the inputs for the AI models. The adaptive neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) models exhibited varying levels of performance across one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) domains. Koeppel et al. [190] combined experiments, FE simulations, and a deep learning (DL) model to predict stresses in 3D printed lattice-cell structures in AM. The approach was validated experimentally, and the simulation data were effectively used to train a long-short-term memory (LSTM) neural network for predictive purposes. Their model achieved a substantial reduction in computational time while maintaining strong agreement with the FE model. Common challenges include time-consuming simulations due to limited computing power and the requirement for extensive simulation data to train the ML model, highlighting this as a vital area for future research.

Chowdhury and Anand [191] proposed a compensation approach using an ANN, in which thermomechanical FE simulation was first used to determine the deformed shape. The ANN was trained on nodal coordinates, learning to map the deformed geometry back to the original design. Once trained, it was able to predict the compensated geometry from the design input. Later, they developed a dual-step approach for optimizing part build orientation and implementing thermal compensation to reduce geometric errors caused by the AM process [192]. First, a weighted optimization model identified the ideal build orientation for a part based on quality and manufacturability metrics. Next, the novel ANN-based geometric compensation method formulated in their previous study [191] was effectively applied to the part in its optimal orientation, making necessary geometric adjustments to mitigate thermal effects from the AM process. Li and Anand [101] developed an ANN approach to predict inherent strains for any selected hatch pattern used in part fabrication. They trained a feedforward neural network using the classical inherent strain method from an initial hatch pattern and validated it with subsequent hatch patterns in mesoscale simulations. The neural network assesses hatch angle relationships

across layers to calculate total inherent strain. Their study showed that the trained neural network accurately predicts inherent strain in random hatch patterns with an error less than 8%.

Hajializadeh and Ince [193] integrated an ANN algorithm with FE analysis to predict residual stress distributions of structural parts fabricated by the directed metal deposition process. In their work, the training dataset originated from FE analysis of 12 layers of structural components and was utilized to train the ANNs. Subsequently, the trained network model was employed to predict residual stress distributions for 18-layered parts. Dong et al. [185] developed a hybrid data-driven framework for LPBF distortion compensation, using experimentally calibrated inherent strains to build a dataset and applying Gaussian Process Regression to generate the compensated geometry. Their model mapped the deformed into nominal geometries using nodal coordinates and could achieve a significant reduction in the maximum distortion up to 80% for both the lattice structure and the canonical part. Vulimiri et al. [194] proposed a bidirectional convolutional long short-term memory neural network surrogate model for predicting residual stress and associated uncertainty in LPBF using a mean–variance estimation framework. Trained on 832 geometries with inherent strain simulations, the model demonstrated strong generalization across complex shapes. It achieved a mean absolute error within 12% of the yield stress and over $20,000\times$ speedup compared to FE analysis, making it highly suitable for rapid design evaluation and optimization applications in AM. Zhang et al. [195] developed an integrated framework combining a simplified FE model, high-resolution residual stress mapping, and ML to efficiently predict and mitigate residual stress distribution in LPBF. Three ML models (multi-layer perceptron, gradient boosting, and random forest regressor) trained on FE data demonstrated good agreement with experimental results. The approach enabled effective inverse distortion compensation, reducing warping in a test sample by 94%.

There is a pressing need to develop a coupled FE and ML framework capable of rapidly predicting inherent strain values as a function of processing parameters and material properties in the LPBF process. Traditional methods rely on computationally expensive thermo-mechanical simulations to determine inherent strains, making them unsuitable for iterative design or optimization workflows. To address this limitation, this study introduces a novel data-driven approach that eliminates the need for mechanical analysis by training five different ML algorithms on inherent strain data obtained from modified inherent strain method-based FE simulations. The mechanical

analysis within detailed thermo-mechanical simulations often encounters significant convergence challenges, particularly when variations in material properties and processing parameters are introduced. While prior studies have primarily addressed only subsets of the influencing factors [101,194,195], the novelty of this research lies in capturing the comprehensive impact of full processing parameter integration and their interaction including laser power, scanning speed, layer thickness, hatching space, and scanning strategy, on inherent strain evolution. Moreover, the proposed framework uniquely combines these key process parameter inputs with other influencing factors including heat source characteristics, material properties, nodal temperatures, nodal depth coordinates, and the number of micron-scale layers to predict inherent strain values both rapidly and accurately. This integrated approach achieves computational speedups of up to 10,000× relative to conventional FE methods. While the FE-generated training data may introduce biases from simplifications like heat source modeling, future enhancements could incorporate experimental measurements for hybrid training to improve real-world accuracy. By enabling fast and accurate inherent strain estimation, this model significantly accelerates residual distortion prediction at the macroscale and thus provides essential guidance for efficient process parameter optimization in LPBF process.

5.2 Methodology

In the following sections, the FE methodology employed in this study, along with the integrated ML algorithms and the evaluation metrics used to assess the predictive performance of the hybrid framework, are described in detail.

5.2.1 Finite element method

A schematic representation of the proposed integrated methodology is illustrated in Fig 5.1, highlighting the coupling between ML and FE analysis. The primary objective of this novel framework is to enable efficient and accurate prediction of inherent strains, thereby reducing computational overhead associated with conventional simulation-based approaches.

The proposed methodology consists of two main steps: (1) FE process simulation, and (2) extraction of FE data for training ML regression models. In the first step, a thermo-mechanical FE simulation is conducted to compute the nodal temperature histories and corresponding inherent strain components (ϵ_{11} , ϵ_{22} , ϵ_{33}) using varying process parameters. These simulation results then serve as the benchmark dataset for training the ML models. The FE simulations are carried out in

Abaqus environment using the modified inherent strain (MIS) approach [30,136], specifically tailored for AM applications. This advanced technique accounts for the layered nature of the process and is structured around two dominant stages that govern residual stress formation and part distortion: The first stage (S_1) corresponds to the time increment during which peak compressive elastic and plastic strains develop near the melt pool. This occurs due to steep thermal gradients and localized softening of the material, wherein the elastic modulus diminishes sharply. The second stage (S_2) pertains to the cooling phase, in which the printed part equilibrates to ambient temperature. During this period, the accumulated mismatch in thermal contraction among successive layers governs the evolution of residual stress [136]. By incorporating both stages, the methodology attempts to capture the layer-wise thermo-mechanical interaction, ensuring that distortion and stress evolution in the lower layers are influenced by the sequential deposition and contraction of the upper layers. The anisotropic inherent strain vector components are derived as a function of thermal and mechanical responses during these stages and are computed as:

$$\varepsilon_{ii}^{inherent} = \varepsilon_{pii}^{s1} + \varepsilon_{eii}^{s1-s2} \quad (\text{Eq 5.1})$$

where, ε_{pii}^{s1} denotes the compressive plastic strain components along the three principal axes ($i=1, 2, 3$) at stage S_1 , while $\varepsilon_{eii}^{s1-s2}$ represents the variation in the elastic strain components between stage S_1 and S_2 along the same directions. Layer configurations spanning 2–11 layers (2L–11L) are considered to reflect different process regimes in the MIS method.

In the second step, the extracted FE data are structured into a dataset suitable for training ML regression models. The input features (i.e. independent variables) include all process parameters, material and heat source types, nodal temperatures, and nodal depth coordinates. For each simulation scenario, nodal temperatures are extracted at stage S_1 . Two types of heat sources, Goldak's double-ellipsoidal and conical-Gaussian, are considered to represent different energy distributions. The materials (Inconel-718 [59,196], Inconel-625 [73,197], and Hastelloy-X [198,199]) are defined using their chemical composition and temperature-dependent physical and mechanical properties at both room and melting temperatures. The dataset is split into training and testing groups for model development and evaluation.

The computational domain for the inherent strain calculation and nodal extraction was considered $300 \mu\text{m} \times 280 \mu\text{m} \times \text{No of micron layers}$. A hexahedral mesh size of $10 \mu\text{m} \times 10 \mu\text{m} \times 5 \mu\text{m}$ with

an 8-node linear heat transfer brick (DC3D8) element type was generated for the thermal simulation. The same mesh size with the 8-node linear brick, reduced integration, hourglass control element type (C3D8R) was also used for the mechanical simulation. Detailed description of the simulation strategy and the definition of boundary conditions are provided in [136,183]. To maintain consistency in the number of input features related to nodal temperature across different simulation cases with varying layer thicknesses, a total of 4,495 nodes were uniformly selected from the central region of the first deposited (bottom) layer. To normalize the influence of layer thickness on the total number of nodes, the model with a 20 μm layer thickness was designated as the reference configuration. In the base case, nodal data were extracted with a resolution of one element per 5 μm along the build direction. For other layer thicknesses, nodal sampling was adjusted accordingly to maintain a comparable distribution density through the height of the part. The details of nodal extraction corresponding to each layer thickness are presented in Table 5.1, where all simulations employed a consistent element size of 5 μm through the thickness of each deposited layer. The dataset comprises 30 experimentally validated simulation cases across parameter ranges: laser power (150–285 W), scan speed (600–1000 mm/s), hatching space (90–140 μm), layer thickness (20–60 μm), and scanning strategies (rotational and non-rotational). The primary processing parameters used for dataset structuring are listed in Table 5.5 in Appendix 5A. The dataset generated for the three different material types were all validated against experimental results. The experimental data for Hastelloy-X were obtained from the literature [119], while those for Inconel-718 and Inconel-625 came from the authors' previous work and literature [27,30,136,183].

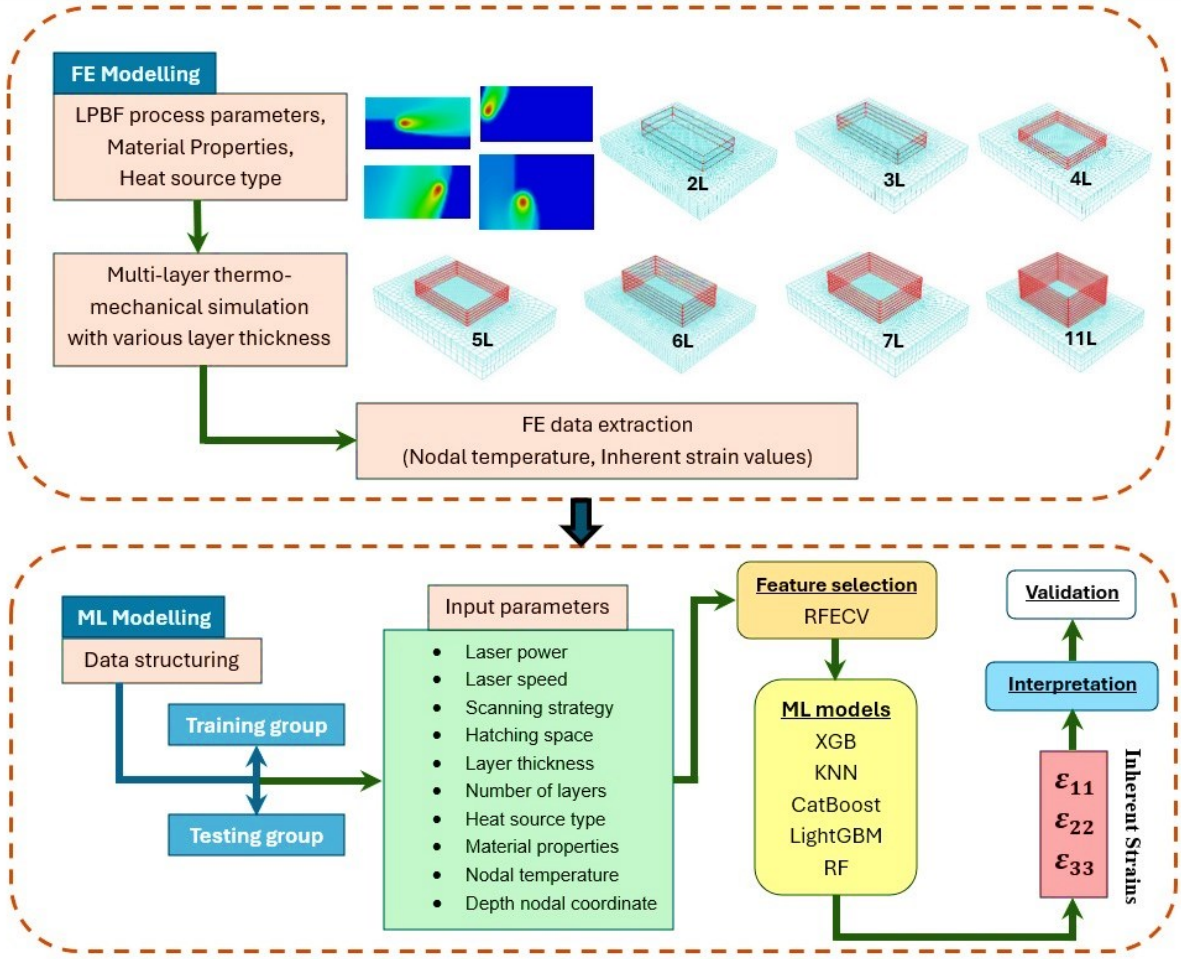


Fig 5.1 Schematic representation of the proposed methodology for predicting inherent strain using an integrated finite element-machine learning framework

Table 5.1 Nodal coordinate of the selected nodes in the build direction (y-coordinate), y_i (μm), for various layer thickness

Layer thickness (μm)	y_1	y_2	y_3	y_4	y_5
20	0	5	10	15	20
30	0	10	15	20	30
40	0	10	20	30	40
60	0	15	30	45	60

5.2.2 Machine learning algorithms

In this work, a preliminary analysis was performed on ten ML and DL algorithms to predict the principal components of the inherent strain tensor and identify the most accurate model for predicting such components. The initial list of methods included multilayer perceptron (MLP)

[200], decision tree (DT) [201], K-nearest neighbors (KNN) [202], random forest (RF) [203], support vector machine (SVM) [204], gradient boosting (GB) [205], extreme gradient boosting (XGB) [206], categorical boosting (CatBoost) [207], adaptive boosting (AdaBoost) [208], and light gradient boosting machine (LightGBM) [209]. Then, the five best-performing methods were identified based on their prediction performance, and their results are presented in the current study. The models selected from this evaluation are briefly discussed in the following section:

Extreme gradient boosting (XGB): XGB is a powerful tree-based ensemble learning method. This technique is known for quick runs, scalability, and high performance on tabular data [206]. XGB is an enhanced version of conventional gradient boosting, renowned for its high accuracy in large-scale datasets. Since it is an ensemble learning technique, it combines multiple weak learners, typically decision trees, using a series of Taylor expansions for accurate optimization of the loss function. XGB aims to iteratively optimize the structure of decision trees by minimizing their residuals. In the structure optimization process, XGB adds a regularization term to the objective function to reduce the probability of overfitting [210]. XGB effectively models complex, non-linear relationships and has demonstrated high predictive accuracy and robustness in various regression and classification tasks, including strain response prediction [211].

Categorical boosting (CatBoost): This categorical boosting algorithm extends gradient boosting method by efficiently handling categorical variables, thus reducing preprocessing requirements and potential data-related errors. It incorporates prediction shift regularization and Bayesian estimation techniques to mitigate overfitting, resulting in improved model robustness and predictive performance [207]. During the training phase, categorical features are encoded into binary representations, which reduces computational complexity. Unlike other ensemble learning algorithms, such as XGB, CatBoost maintains a symmetric structure with uniform decision tree depth across all nodes [212].

Light gradient boosting machine (LightGBM): This is an efficient and scalable gradient boosting algorithm optimized for speed and memory usage. It constructs decision trees using a leaf-wise growth strategy, allowing multiple leaves at the same depth to split simultaneously for faster, parallel training [213]. LightGBM enhances computational efficiency by pre-calculation of feature histograms, column randomization, and bootstrapped subsampling. The methodologies,

along with comprehensive hyperparameter tuning possibilities, provide LightGBM with an adaptable and potent model for many ML applications [214].

K-nearest neighbors (KNN): This is a simple and non-parametric algorithm for classification and regression. KNN understands the concept of similarity, making predictions and classifications based on the closeness of data points in the feature space [202]. KNN can face significant difficulties related to computation cost and memory. However, the cost and performance can be improved through preprocessing, feature selection, and hyperparameter tuning [215]. KNN is highly effective for small datasets with a few observations, without requiring strict parametric assumptions [216].

Random forest (RF): This is a widely used ensemble learning method for classification and regression, esteemed for its precision and robustness. It generates several decision trees using bootstrap samples and combines their predictions via majority voting or averaging [203]. RF randomizes data sample and feature selection, reducing overfitting and improving generalization. It also gives reasonable metrics for the importance of any features in the model, which is a nice exploratory tool. However, because of the mixed-effect of self-aggregating ensemble nature, it is less interpretable as a model, and it can be computationally demanding with often many trees [217].

5.2.3 Feature selection

The dataset includes 9024 input features. Since the number of features is significant, the ML models are prone to overfitting [218]. Further, increasing the number of features increases the computational cost, which is a major concern in modeling large-scale datasets. To address these, we applied two approaches to optimize the input features in the modeling. First, the nodal coordinates located at the bottom of the samples were excluded, as their y-coordinate value was consistently zero and, therefore, did not contribute any informative learning signal. Following this preprocessing step, a total of 8125 features remained. Second, we applied a robust feature selection technique to identify the optimal feature set. Feature selection techniques filter out irrelevant or unnecessary features, which can increase the prediction performance, reduce computational cost and complexity, and prevent overfitting [217].

For this purpose, the recursive feature elimination with cross-validation (RFECV) is applied to iteratively remove the least important features while conducting an automatic tuning of the selected features to improve the model performance through the cross-validation technique [219,220]. The method involves partitioning the dataset into k subsets. The model is then trained using $k-1$ folds and evaluated on the remaining fold. This approach is executed k times, ensuring that each subset serves as the test set once. Finally, an average value of performance metrics over all folds is used to identify the optimal feature set. At each iteration, a given number of less important features are removed, and that number is called a step. We run the model for different step sizes from 1 to 50 to identify the optimal step size of RFECV for each dependent variable. RFECV reduces dimensionality and computational expense while preventing overfitting by removing unnecessary features, thereby improving the prediction performance.

After identifying the optimal feature set for each dependent variable (i.e., the inherent strain components), the data is randomly divided into two parts: a training set (80% of observations) and a testing set (the remaining 20%). The training data is used to train and tune ML techniques. The testing set is applied to evaluate the prediction performance of the model on unseen data. To tune hyperparameters of each ML model, Optuna and k -fold cross-validation (considering $k=5$) are employed. Optuna is a powerful tuning technique, which is renowned for its quick processing, efficient pruning strategies, and dynamic construction of parameter search spaces. This method iteratively uses Bayesian optimization to tune the hyperparameters [221]. The optimized hyperparameters obtained after the tuning process for each ML algorithm are summarized in Table 5.6 to Table 5.8 in Appendix B.

5.2.4 Model evaluation

After tuning the ML models, their performance was evaluated on testing data by the merit indicators presented in Table 5.2. In the formulations, $y, \hat{y}, \bar{y}, n$, and k are the actual value, predicted value, the mean of all observed values y_i , number of samples, and number of model parameters, respectively.

Shapley Additive Explanation (SHAP) was then applied to calculate the relative influence of input features on the dependent variables. SHAP is a feature-based interpretability method that provides global and local explanations, which was developed by Lundberg and Lee [222]. It serves as an interpretation technique that synchronizes with a prediction method and sorts independent

variables based on their relative influence on the dependent variable. For this purpose, SHAP utilizes a game theory approach and evaluates relative influences using a unitless measure called the Shapley value [223]. In this study, after identifying the best-performing model on each dependent variable, it is synchronized with SHAP to prioritize the variables based on their importance on the inherent strains.

Finally, to validate the developed ML models for the distortion prediction, two unseen examples are fed into the model to evaluate its generalization capability. The predicted inherent strains are then integrated into the macroscale cantilever beam simulation to predict residual distortion, with the model's accuracy evaluated through comparison against experimentally measured distortion. Fig 5.2 shows the fabricated cantilever beams (AMBench2018 challenge proposed by NIST [120]) for Inconel-718 with various process parameters, along with the optical scan distortion analyzer. The samples were printed with EOS M290 and RENISHAW AM 400 LPBF machines. After fabrication, the support was cut 3 mm above the substrate, causing the cantilever to bend upward due to residual stress. Distortion was measured using optical scanning before and after support removal.

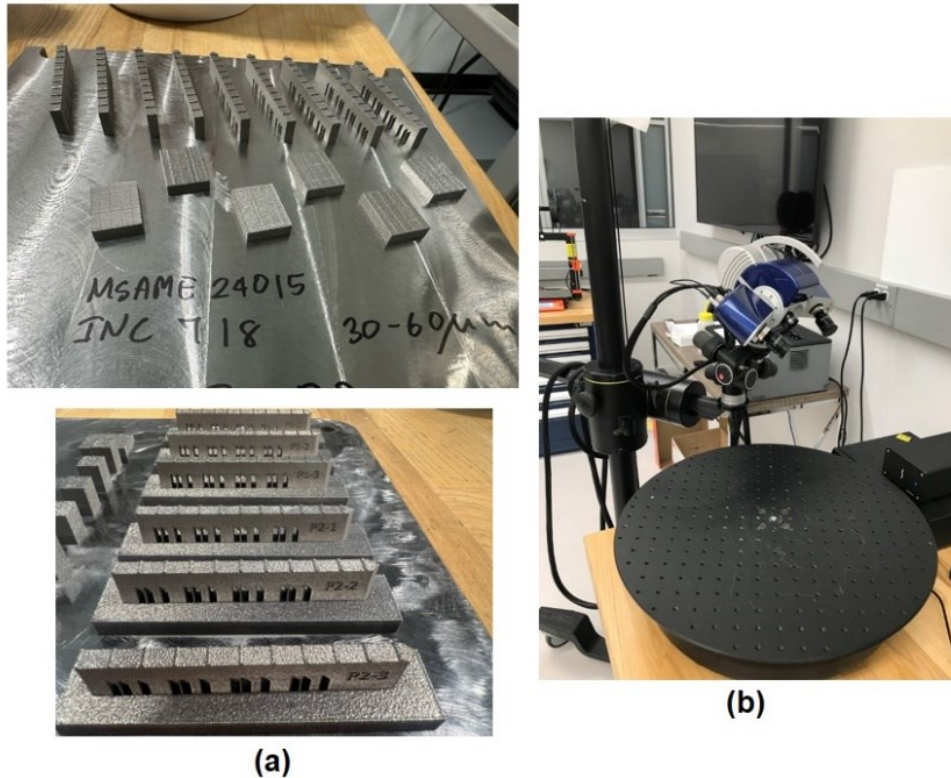


Fig 5.2 (a) Printed cantilever beams for Inconel-718; (b) Optical scan distortion analyzer

Table 5.2 Performance metrics and their mathematical formulations

Indicator	Description	Formula
R^2 (Coefficient of determination)	Measures of how well the predicted values explain the variability of the observed data (higher values are better)	$1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$
MAE (Mean absolute error)	Average magnitude of prediction errors, regardless of direction. (lower values are better)	$\frac{1}{n} \sum_{i=1}^n y_i - \hat{y}_i $
MSE (Mean squared error)	Average of squared prediction errors, giving more weight to larger errors (lower values are better)	$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$
AIC (Akaike information criterion)	Measures model quality considering goodness-of-fit and model complexity; (lower values indicate a better trade-off)	$2k + n \ln \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}$
EV (Explained variance)	Proportion of variance in the target variable explained by the model's predictions (higher values are better)	$1 - \frac{\text{var}(y - \hat{y})}{\text{var}(y)}$
NMAE (Normalized mean absolute error)	The ratio of MAE to the average of actual values	$\frac{\frac{1}{n} \sum_{i=1}^n y_i - \hat{y}_i }{\frac{1}{n} \sum_{i=1}^n (y_i)}$

5.3 Results and discussion

In the subsequent sections, the results of the thermo-mechanical FE simulations used for data structuring are first presented. This is followed by a detailed explanation of the optimal feature selection process and its corresponding outcomes. Finally, the predictive performance of the developed model is analyzed and interpreted comprehensively, and its validity is assessed using unseen data to evaluate its generalization capability.

5.3.1 Detailed thermo-mechanical simulation

A comprehensive thermo-mechanical FE campaign was conducted for 30 experimentally validated cases to generate the dataset required for training the ML models. While the number of observations is relatively small, this limitation is offset by the high fidelity of the data, which are directly representative of physically realizable process conditions. Accurate thermal simulations

in laser-based manufacturing require precise melt pool dimensions and heat source parameters; therefore, the use of artificially generated data or non-physical process parameters was not pursued to maintain strict physical consistency. Model training was based on thermally consistent simulation results that preserved experimentally validated melt pool characteristics, from which nodal temperature histories were extracted over a specified time interval to augment the feature space. By constraining the training data to experimentally validated conditions, the resulting model is expected to generalize more reliably within the physically meaningful parameter space.

These FE simulations were employed to extract nodal temperatures corresponding to the S_I stage and subsequently compute inherent strains via the MIS method. As outlined previously, the number of layers required to define the S_I period is strongly influenced by both the material properties and the processing parameters. The melting temperatures of Inconel-625, Inconel-718, and Hastelloy-X are 1320 °C, 1337 °C, and 1307 °C, respectively. Accordingly, the minimum number of layers was determined based on the heating and cooling cycles of the first layer up to the onset of melting. Fig 5.3 presents the thermal histories of the bottom layer for six representative cases. Distinct temperature peaks are observed in each case, followed by rapid cooling associated with the powder recoating step inherent to the LPBF process. Results clearly show that the temperature profiles are influenced not only by the process parameters but also by the material type. In other words, different material types and variations in process parameters lead to distinct thermal cycling histories and require a different number of layers to define the intermediate stage used for nodal temperature extraction and dataset construction. The thermal histories were extracted directly from the Abaqus output database using a MATLAB code developed by Papazafeiropoulos et al. [224]. Then, the mechanical analysis was performed on each case to calculate the inherent strains.

5.3.2 Optimal variable selection

As mentioned in the preceding section, the step size (the number of features removed at each iteration) of RFECV was optimized for each dependent variable. The optimal step size for ε_{11} , ε_{22} , and ε_{33} was found to be 20, 1, and 10, respectively. Following this optimization, RFECV was applied to the dataset, which comprised 8125 features. The resulting optimal feature subsets contained 4846, 6157, and 6268 features for ε_{11} , ε_{22} , and ε_{33} , respectively. For each dependent variable, the category of selected features was investigated, and the percentage of remaining features for each category of features is illustrated in Fig 5.4. It can be seen that the material type

and process parameter categories retain almost identical proportions across all strain components, whereas the nodal temperature and nodal coordinate categories vary. This variation arises from the dependence of nodal temperature on process parameters and material properties, leading to greater feature elimination and differing retention rates among strains. The nodal temperature and nodal coordinate were grouped in the same category because of their direct relationship, wherein each coordinate is intrinsically associated with a corresponding temperature.

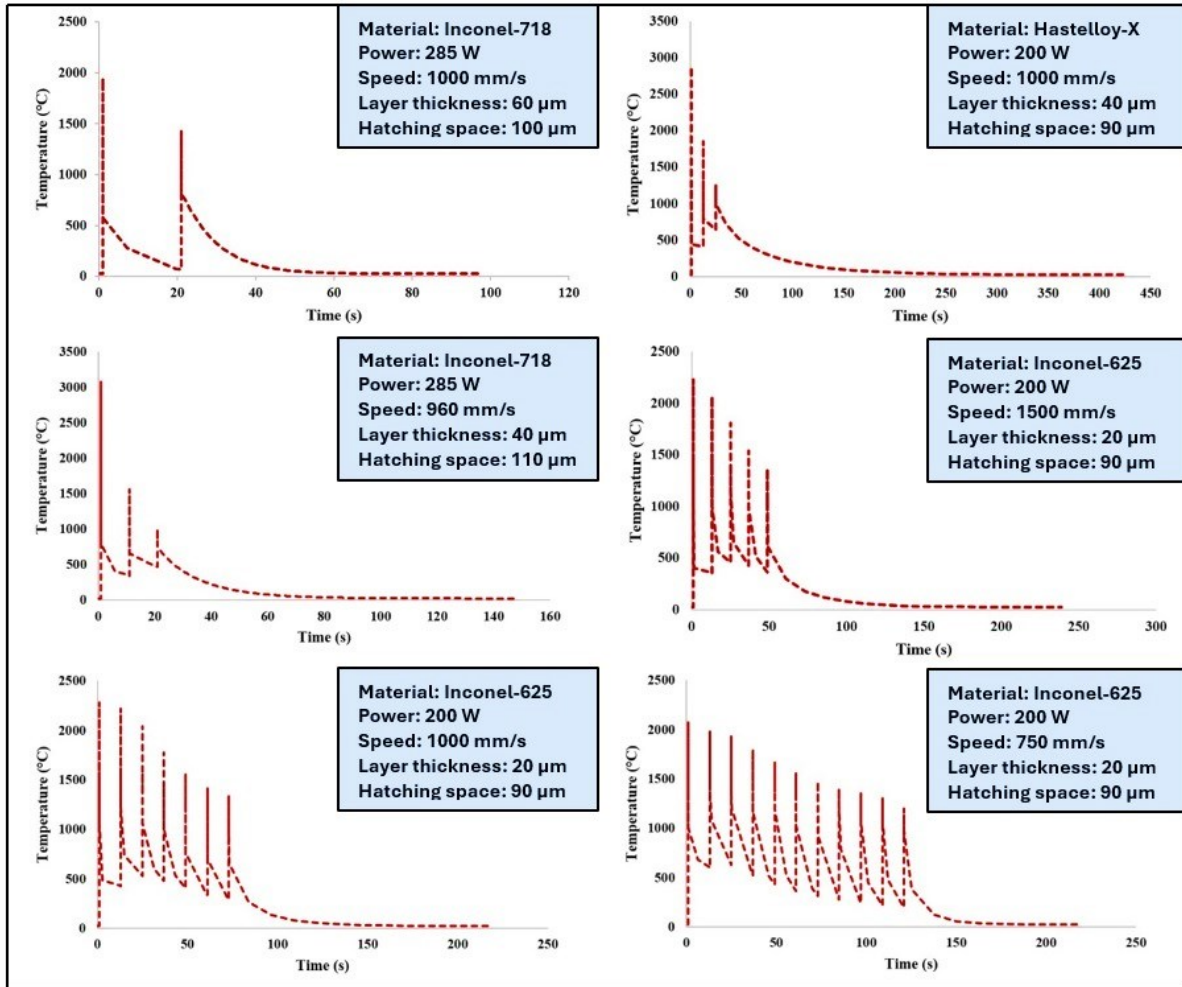


Fig 5.3 Thermal history at a random element on the 1st layer for six representative cases

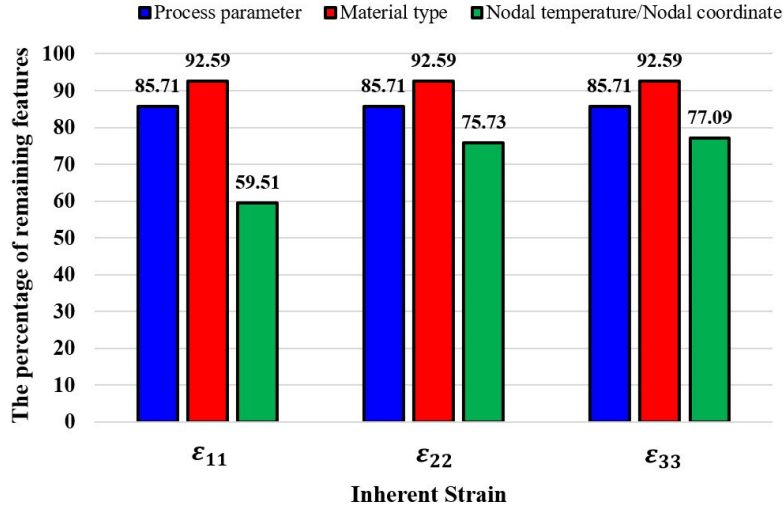


Fig 5.4 The percentage of remaining features for each category of features and each strain

5.3.3 Model performance analysis

Table 5.3 summarizes the predictive performance of five ML algorithms on the testing set for three dependent variables (ϵ_{11} , ϵ_{22} , ϵ_{33}), using R^2 , MAE, MSE, AIC, and EV as evaluation metrics.

For ϵ_{11} , CatBoost achieved the most favorable results across nearly all indicators. It obtained the highest R^2 (0.918), the lowest MAE (0.00221), the lowest MSE (8.53×10^{-6}), the lowest AIC (-52.4), and the highest EV (0.756). These values indicate excellent predictive accuracy, minimal error magnitude, and a strong trade-off between fit quality and model complexity. XGB also performed competitively, particularly in terms of MAE (0.00256) and EV (0.689).

For ϵ_{22} , KNN achieved the lowest MAE (0.0028) and the lowest MSE (1.54×10^{-5}), outperforming other models in terms of absolute error minimization. XGB followed closely with competitive MAE (0.00694) and a moderate R^2 (0.543). Negative EV values for RF and LightGBM reflect poor variance explanation, suggesting that these models were unable to capture the underlying data distribution effectively for this variable. For ϵ_{33} , KNN again achieved the lowest MAE (0.00248) and the lowest MSE (8.15×10^{-6}), indicating superior performance in minimizing prediction errors. However, in terms of R^2 , XGB emerged as the top performer (0.882), despite its negative EV and higher MAE. CatBoost and LightGBM exhibited substantially lower performance for this variable. It should be noted that the R^2 primarily evaluates correlation and trend capture, without directly assessing prediction error magnitude. Accordingly, MAE provides a more explicit measure of accuracy, revealing that for ϵ_{22} and ϵ_{33} , KNN outperforms XGB despite its lower R^2 values.

Although the strain components are governed by the same physical mechanisms, their statistical characteristics differ, motivating the use of different learning algorithms. The ε_{11} component exhibits higher variance, noticeable skewness, and stronger sensitivity to process parameters and nodal temperature, indicating pronounced nonlinear behavior that is best captured by CatBoost. In contrast, ε_{22} and ε_{33} show lower variance, near-symmetric distributions, and smoother response surfaces, making them better suited to prediction using the local interpolation characteristics of the KNN algorithm.

Overall, the results demonstrate that the error-based (e.g., MAE) ranking sometimes differs from R^2 -based ranking. While CatBoost excelled for ε_{11} , KNN was superior for ε_{22} and ε_{33} in terms of minimizing absolute prediction errors. The findings emphasize that model selection in predictive modeling should be driven by a multi-metric evaluation framework, since various algorithms may perform optimally under distinct performance criteria based on the properties of the target variable.

To provide a clearer perspective on the relative prediction errors of the best-performing models, the normalized mean absolute error (NMAE) was computed and is presented in Fig 5.5. The resulting relative errors for ε_{11} , ε_{22} , and ε_{33} were 16.5%, 16.3%, and 22.5%, respectively, in comparison with the full multi-scale FE simulations. By increasing the number of observations, prediction errors could potentially be reduced for all dependent variables [225].

Table 5.3 Statistical performances of different ML algorithms on testing data

Dependent variable	Model	R^2	MAE	MSE	AIC	EV
ε_{11}	KNN	0.551	0.00317	1.72×10^{-5}	-48.9	0.549
	RF	0.551	0.00344	1.75×10^{-5}	-48.8	0.498
	XGB	0.690	0.00256	1.09×10^{-5}	-51.1	0.689
	CatBoost	0.918	0.00221	8.53×10^{-6}	-52.4	0.756
	LightGBM	0.635	0.00224	1.59×10^{-5}	-43.2	0.630
ε_{22}	KNN	0.493	0.00280	1.54×10^{-5}	-49.4	0.385
	RF	0.010	0.00731	7.78×10^{-5}	-41.3	-0.001
	XGB	0.543	0.00694	8.00×10^{-5}	-41.2	-1.716
	CatBoost	0.169	0.00487	4.13×10^{-5}	-44.5	0.054
	LightGBM	0.005	0.00727	9.67×10^{-5}	-34.2	-0.805
ε_{33}	KNN	0.669	0.00248	8.15×10^{-6}	-52.6	0.650
	RF	0.719	0.00568	3.53×10^{-5}	-45.3	-0.520
	XGB	0.882	0.00857	1.04×10^{-4}	-39.8	-3.072
	CatBoost	0.017	0.00389	3.62×10^{-5}	-45.1	-0.435
	LightGBM	0.202	0.00442	2.61×10^{-5}	-40.8	-0.019

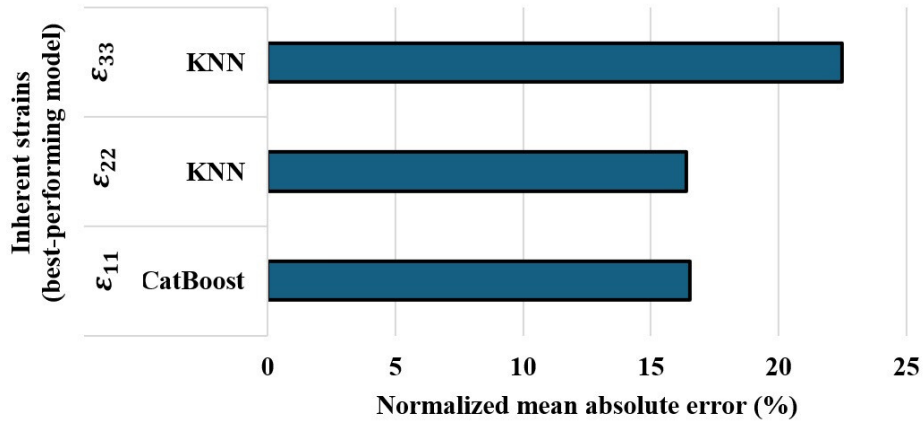


Fig 5.5 The NMAE of the best-performing models on testing data

Fig 5.6 depicts error histogram violin plots of residual percentages for the ML models applied to the testing dataset of ε_{11} , ε_{22} , and ε_{33} . Each violin plot illustrates the distribution of percentage residuals for the five models. In these plots, the vertical axis shows residual percentages; values closer to zero indicate better predictive accuracy, while shorter violin lengths reflect a narrower error range and, consequently, lower variance in model predictions. Further, the width of each violin shows the density of residuals, and a wide section represents a greater density of residuals in that range, and a narrow section denotes a lower density of residuals in that range. Therefore, having a wide range of residuals near zero implies the superiority of a model. The black bar in the middle of each violin presents the interquartile range (25% and 75% quartiles), and having these values near zero indicates more stable and accurate predictions.

For ε_{11} , CatBoost demonstrates one of the most favorable performances, with residuals tightly distributed between -40% and 20% , indicating both low error magnitude and limited variability. Moreover, the widest section is almost located very close to the zero indicator, meaning that the highest frequency of residuals is centered around zero. Regarding interquartile ranges, CatBoost has the smallest residuals at the upper quartile (75%), while KNN shows minimum residuals at the lower quartile (25%). For ε_{22} , KNN exhibits the narrowest residual range, suggesting consistent predictions with limited extreme deviations. Further, the 25% and 75% quartiles of KNN are centered around zero, indicating that the KNN can predict the ε_{22} of 50% of observations with a residual of almost zero. The positions of the upper and lower quartiles (25% and 75%) near zero indicate stable prediction performance and a lower risk of predictions with significant residuals. On the other hand, the residual range of LightGBM, XGB, and RF is much wider than KNN, and

they predict the ε_{22} of some observations with a significant residual. Moreover, the density of KNN residuals (width) around zero is maximum, indicating a superior performance of KNN in predicting ε_{22} . Similarly, for ε_{33} , KNN again achieves the shortest violin span, signifying both accuracy and stability across predictions. The residual of KNN on testing data ranged between +25 to -35, and this range is much shorter than that of other methods. CatBoost has the best performance in terms of interquartile range (the most compact 25%–75%), but it has a significant range, indicating much lower stability than KNN. These results align with the trends observed in MAE and MSE in Table 5.3, underscoring the importance of a multi-metric evaluation framework for effective model selection.

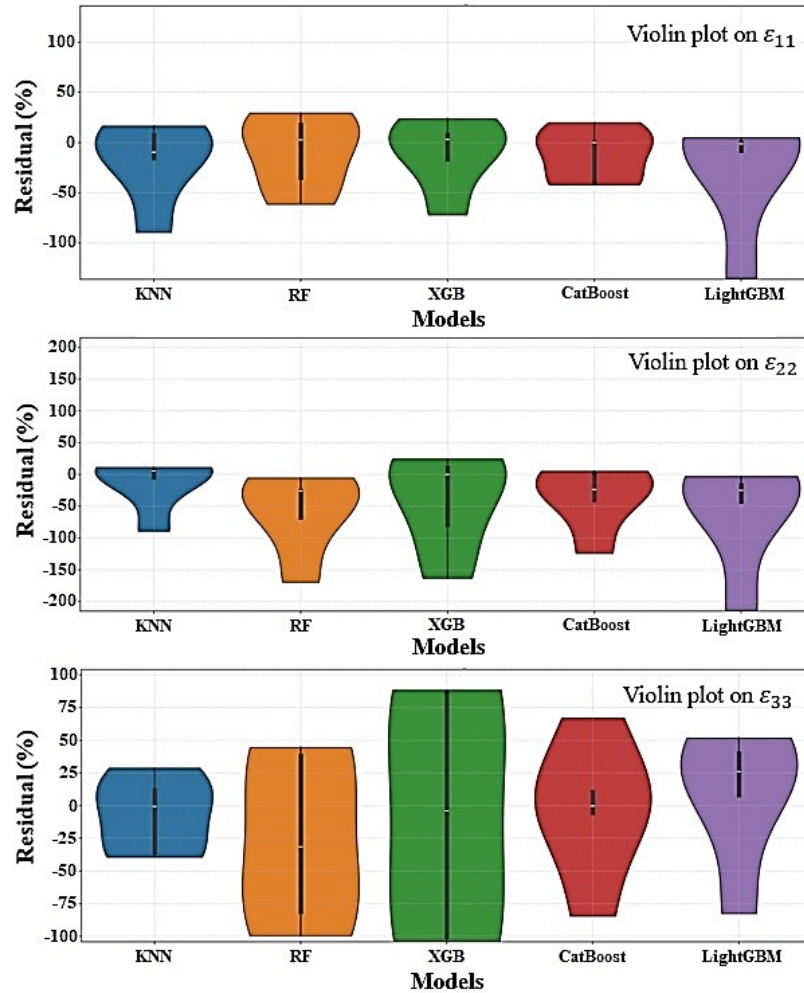


Fig 5.6 The distribution of residuals for different ML models

The SHAP analysis is performed to investigate the relative influence of each optimal category on dependent variables (ε_{11} , ε_{22} , and ε_{33}). To do so, variables are grouped by category, and the SHAP

values within each group are summed. Then, the average SHAP values of each group over the dependent variables are calculated. Fig 5.7 illustrates the contribution of nodal temperature, process parameters, material type, and nodal coordinate to the model's predictive accuracy, expressed as the percentage of average SHAP values across all dependent variables. The results indicate that material type and process parameters dominate the model's explanatory power, collectively accounting for nearly 70% of the influence. The third crucial factor is nodal temperature, which shows an indirect correlation with both process parameters and material type. Its importance is particularly evident in model performance as variations in process parameters and layer thickness alter the number of micron-scale layers, thereby affecting the local thermal response, which has also been reported in previous studies [108,119]. Lastly, the nodal coordinate shows a relatively minor effect on inherent strains.

To further highlight the prominent role of nodal temperature in the model, Fig 8 presents a SHAP bee swarm summary plot of the 20 most influential input parameters contributing to the prediction of the inherent strain components ε_{11} , ε_{22} , and ε_{33} . Each point represents an individual sample, and the features are ranked in descending order according to their mean absolute SHAP values. The vertical gray line denotes zero contribution, separating positive and negative impacts on the model output. Points located to the right of this line indicate an increase in the predicted strain components, whereas points located to the left indicate a decrease. The color scale (at the right of plots) represents the value of the corresponding input feature, with red and blue denoting high and low values, respectively. Across the SHAP summary plots corresponding to the three inherent strain components, the nodal temperature features (NT) consistently dominate the ranked list of influential inputs and exhibit the largest distributions of absolute SHAP values. The pronounced horizontal spread of the NT features, relative to the remaining process parameters, indicates that local thermal states in the computational domain exert the strongest contribution to the model output. These results confirm that the nodal temperature field, which implicitly captures the combined effects of material properties and process parameters, is the primary driver governing the prediction of inherent strain components in the model.

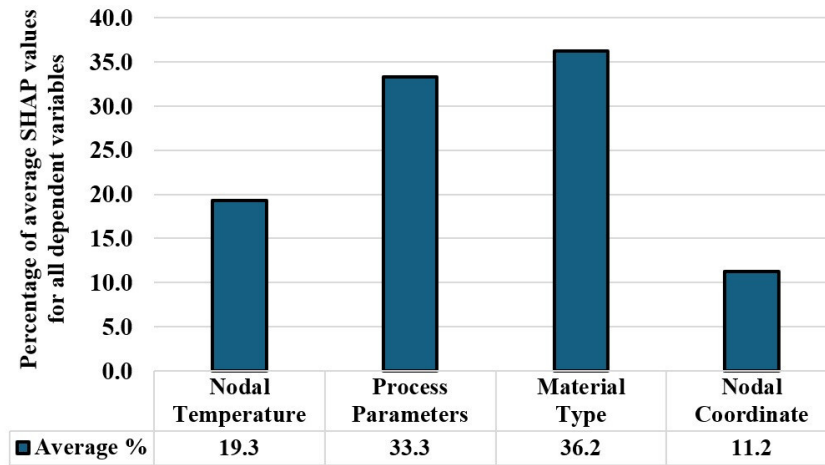
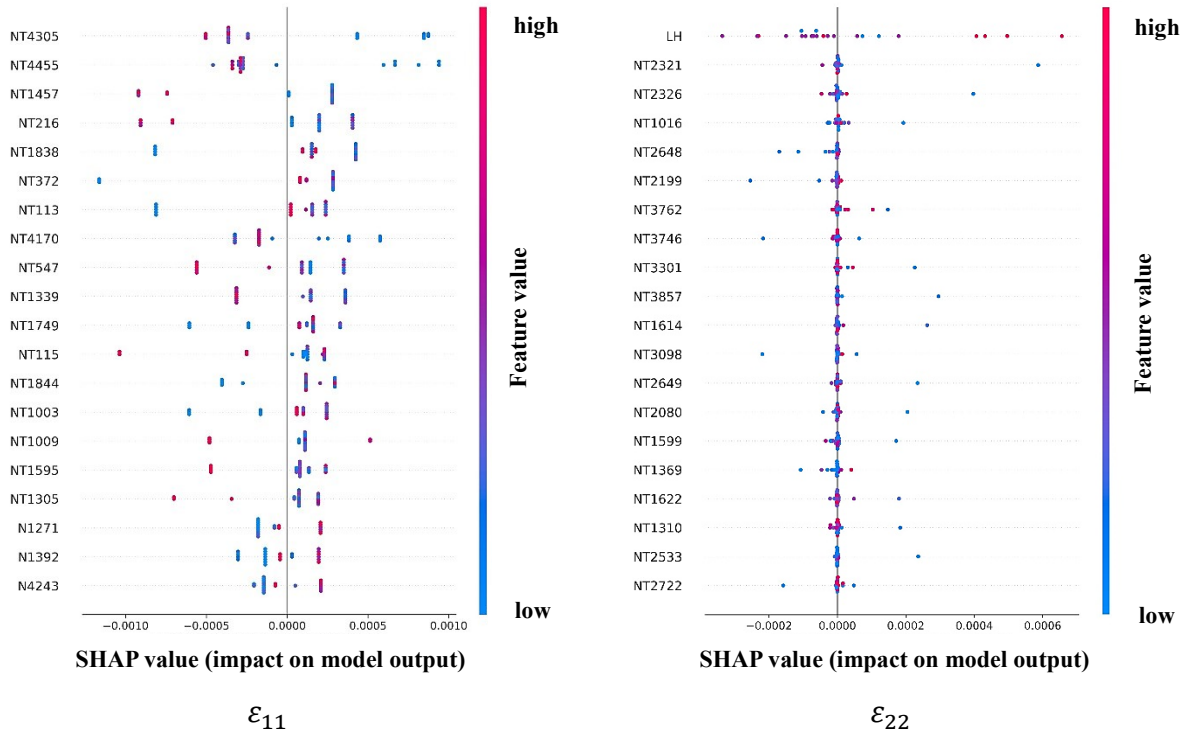


Fig 5.7 The summation of average SHAP values on dependent variables for features in each category



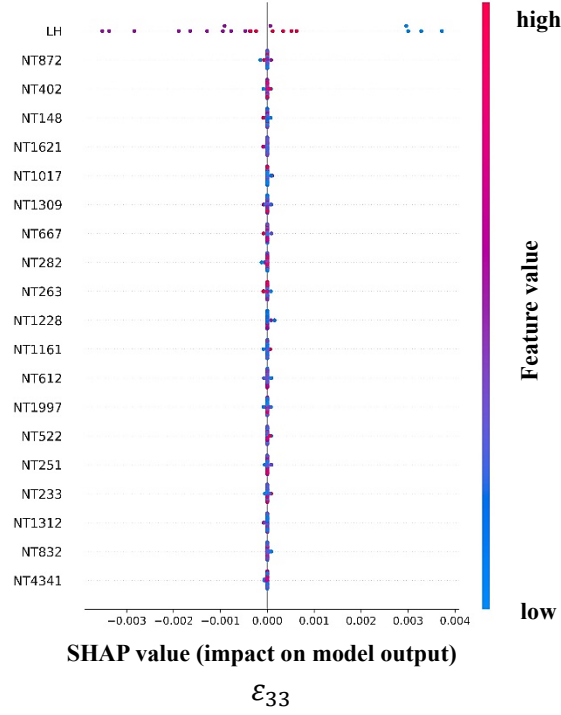


Fig 8 The SHAP bee swarm plots of the top 20 input features for predicting the inherent strain components. Nodal temperature (NT), Latent heat (LH), Nodal coordinate (N)

5.3.4 Model validation

Table 5.4 presents the maximum distortion values measured using the optical scan distortion analyzer for the fabricated Inconel-718 cantilever beams. Among these specimens, cases 2 and 5 were selected as unseen datasets to assess the model’s validation performance and its generalization capability. The discrete variable S denotes the scanning pattern, with values of 1 and 2 corresponding to the non-rotational and rotational strategies, respectively. The experimental measurements were conducted on cantilever beams at 11 ridge points as illustrated in Fig 5.9. Among these, ridge point 11 showed the highest distortion after support removal, making it the critical reference for the model validation. The model predicted the inherent strain vectors as $(\epsilon_{11} = -0.0019, \epsilon_{22} = 0.0028, \epsilon_{33} = -0.0018)$ and $(\epsilon_{11} = -0.0158, \epsilon_{22} = 0.0233, \epsilon_{33} = -0.0032)$ for the cases 2 and 5, respectively. These strains were then applied to calculate the cantilever beam distortion. As shown in Fig 5.10, the maximum predicted distortion at ridge point 11 was 0.56 and 2.10 mm for cases 2 and 5, respectively, yielding errors of about 11% and 16% relative to the experimental results, which remain within the acceptable range. Further details of the macroscale simulation based on the agglomeration technique can be found in our previous publications [136,183].

The proposed hybrid FE–ML framework enables rapid and accurate prediction of inherent strains across diverse LPBF conditions. It also dramatically reduces computational time between 8,000–10,000× (depending on the process parameters) compared to full-scale simulations while maintaining physical fidelity, making it suitable for optimization and distortion control in AM design. With respect to generalization, the proposed model ensures that when new observations fall within the range of input parameters used during training, the inherent strain components can be predicted with acceptable accuracy. In cases where new observations lie outside the original training domain, the same methodological framework must be applied to retrain the model, thereby enabling reliable prediction of the corresponding strain values.

Table 5.4 Process parameters with experimental measurement

Case	P (W)	V (mm/s)	Hs (μm)	S	t (μm)	Max Distortion from Experiment (mm)
1	200	600	140	1	60	0.895
2	200	600	140	2	60	0.502
3	220	1000	140	1	60	0.733
4	220	1000	140	2	60	0.712
5	285	1000	100	1	30	1.799
6	285	1000	100	2	30	1.025
7	150	900	90	2	30	0.344
8	200	1000	90	2	30	0.335
9	250	1000	100	2	60	0.414

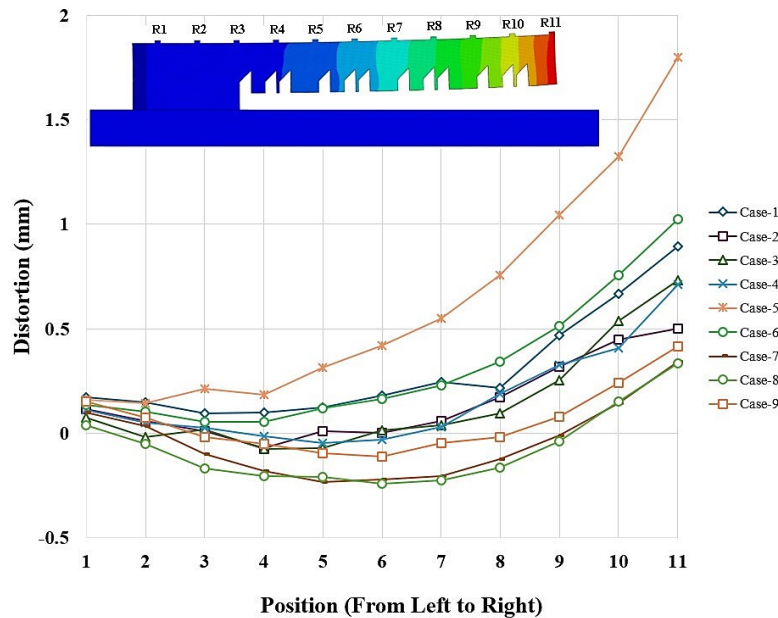


Fig 5.9 Distortion measurement for the fabricated cantilever beams after support removal

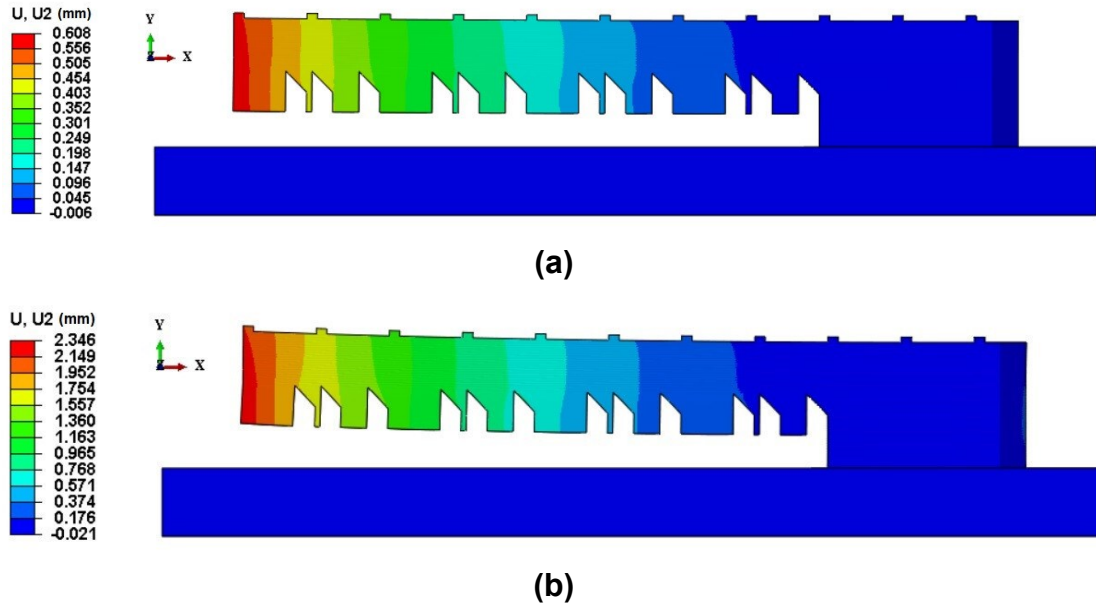


Fig 5.10 Distortion prediction in Abaqus based on inherent strains derived from ML model; a) Case 2, b) Case 5

5.4 Conclusions and future remarks

In this study, an integrated FE–ML framework was developed to significantly reduce the computational time required for inherent strain calculation and, consequently, residual distortion prediction across different process parameters and material types. Five ML algorithms including, XGBoost, CatBoost, LightGBM, KNN, and RF, were evaluated for their predictive capability of inherent strains. The models were trained and tested using a dataset derived from experimentally validated numerical simulations, and their performance was further verified against an independent experimental case involving the distortion prediction of a cantilever beam (NIST AMBench2018). Key findings of this research are presented as follows:

- Among the selected ML models, Catboost, and KNN showed their best performance for inherent strains prediction with an average mean absolute error of 16.5 %, 16.3 %, and 22.5 %, for ε_{11} , ε_{22} , and ε_{33} , respectively.
- The feature selection (RFECV) could reduce dimensionality of the dataset and computational cost while improving the model's prediction performance.
- The relative influence of each feature category on inherent strains was assessed using SHAP analysis. The results revealed that material type and process parameters were the most influential factors, whereas nodal temperature exhibited an indirect effect on the dependent variables, contributing approximately 19% within the developed model.

- Model validation was performed on two unseen datasets and could achieve the error up to 16 % for residual distortion prediction of the cantilever beam compared with experimental measurements.
- The developed hybrid model could speed up the inherent strains calculation up to 10,000× compared to multi-scale FE simulations [136].

This study highlights the role of data-driven analysis in residual distortion prediction and demonstrates that integrating ML with FE can substantially improve computational efficiency in LPBF. While the FE-generated training data may introduce biases from simplifications, such as heat-source modeling, future enhancements could incorporate experimental measurements (in-situ temperature profiles or strain gauges) to improve hybrid training and real-world accuracy. These biases are particularly pronounced for materials with varying thermal conductivities or phase transformations, such as titanium alloys, necessitating robust calibration against experimental data. We incorporate material properties (thermal conductivity, yield strength) as explicit inputs to improve the model's adaptability to various alloys. Future work will validate the model on Ti-6Al-4V, which poses challenges due to its lower heat dissipation, and on lattice geometries to support complex AM designs. Model accuracy could be further improved by expanding the training dataset. Future work should also focus on developing digital twin frameworks, potentially leveraging physics-informed neural networks (PINNs) to predict inherent strains without relying on thermal simulations, thereby advancing real-time process optimization.

Appendix 5A Processing parameters used to structure the ML dataset

Table 5.5 Experimentally-validated processing parameters used for structuring dataset

Laser Power (W)	Laser Velocity (mm/s)	Scanning Strategy	Hatching Space (μm)	Layer Thickness (μm)	Material Type	No of Layers
200	600	Rotational (90°)	140	60	Inconel-718	2
285	960	Rotational (90°)	110	40	Inconel-718	3
200	1000	Non-Rotational (0°)	90	20	Inconel-625	7
150	1000	Non-Rotational (0°)	90	40	Hastelloy-X	2
285	1000	Rotational (90°)	100	30	Inconel-718	2
285	1000	Non-Rotational (0°)	100	30	Inconel-718	2
100	1000	Non-Rotational (0°)	90	20	Inconel-625	4
100	1000	Rotational (90°)	90	20	Inconel-625	4
200	1000	Rotational (90°)	90	20	Inconel-625	7
200	1000	Non-Rotational (0°)	90	40	Hastelloy-X	3
200	1000	Non-Rotational (0°)	90	30	Inconel-718	6
285	960	Non-Rotational (0°)	110	40	Inconel-718	3
250	1000	Rotational (90°)	100	60	Inconel-718	3
200	1000	Rotational (90°)	90	30	Inconel-718	6
150	1000	Rotational (90°)	100	20	Hastelloy-X	3
250	1000	Non-Rotational (0°)	100	60	Inconel-718	3
200	750	Non-Rotational (0°)	90	20	Inconel-625	11
200	1500	Non-Rotational (0°)	90	20	Inconel-625	5
285	1000	Rotational (67°)	100	60	Inconel-718	2
200	600	Non-Rotational (0°)	140	60	Inconel-718	2
150	1000	Non-Rotational (0°)	100	20	Hastelloy-X	3
150	900	Rotational (90°)	90	30	Inconel-718	6
150	1000	Rotational (67°)	100	20	Hastelloy-X	6
150	1000	Rotational (67°)	90	40	Hastelloy-X	5
100	1000	Rotational (67°)	90	20	Inconel-625	7
200	1500	Rotational (67°)	90	20	Inconel-625	7
200	1000	Rotational (67°)	90	20	Inconel-625	7

285	960	Rotational (67°)	110	40	Inconel-718	3
200	750	Rotational (67°)	90	20	Inconel-625	11
200	1000	Rotational (67°)	90	40	Hastelloy-X	3

Appendix 5B Optimized hyperparameters after tuning process

Table 5.6 Optimized hyperparameters for ML algorithms for ε_{11}

Algorithms		XGBoost	CatBoost	LightGBM	RF	KNN
Hyperparameter	Definition	Value/Type				
Learning rate	The step size	0.1710	0.2925	0.1135	-	-
Maximum depth	The maximum depth of DTs	3	3	13	16	-
Number of estimators	Number of weak learners (DTs)	361	340	742	382	-
Minimum samples split	The minimum number of observations needed to split a node	-	-	-	7	-
K	Number of neighbors	-	-	-	-	3
Weights	The weight of neighbors in prediction	-	-	-	-	distance
P	Power parameter for the distance	-	-	-	-	1

Table 5.7 Optimized hyperparameters for ML algorithms for ε_{22}

Algorithms		XGBoost	CatBoost	LightGBM	RF	KNN
Hyperparameter	Definition	Value/Type				
Learning rate	The step size	0.0102	0.3608	0.1987	-	-
Maximum depth	The maximum depth of DTs	9	5	12	24	-
Number of estimators	Number of weak learners (DTs)	101	455	500	378	-
Minimum samples split	The minimum number of observations needed to split a node	-	-	-	8	-
K	Number of neighbors	-	-	-	-	10
Weights	The weight of neighbors in prediction	-	-	-	-	distance
P	Power parameter for the distance	-	-	-	-	1

Table 5.8 Optimized hyperparameters for ML algorithms for ε_{33}

Algorithms		XGBoost	CatBoost	LightGBM	RF	KNN
Hyperparameter	Definition	Value/Type				
Learning rate	The step size	0.3554	0.2028	0.0305	-	-
Maximum depth	The maximum depth of DTs	7	5	5	8	-
Number of estimators	Number of weak learners (DTs)	247	518	731	463	-
Minimum samples split	The minimum number of observations needed to split a node	-	-	-	7	-
K	Number of neighbors	-	-	-	-	5
Weights	The weight of neighbors in prediction	-	-	-	-	uniform
P	Power parameter for the distance	-	-	-	-	2

Chapter 6 Conclusions, and future work

6.1 Summary and conclusions

The primary objective of this research study was to develop a high-fidelity, experimentally validated FE framework capable of accurately predicting the residual stresses and distortions in components manufactured by the LPBF process. Due to the influence of various process parameters on final distortions in LPBF process and also inherent computational cost associated with high-fidelity FE model, this study also sought to accelerate these predictions by employing FE-based surrogate modeling combined with data-driven approaches. Ultimately, the proposed framework integrates robust FE analysis with ML algorithms to improve both the computational efficiency and predictive accuracy of residual stress and distortion simulations in LPBF-fabricated parts.

To achieve this, a comprehensive literature review on the thermo-mechanical modeling of the LPBF, with emphasis on IS and MIS methodologies, was first conducted. Building on this foundation, process simulation with a focus on the MIS methodology was performed in Abaqus. In this phase, a sequentially coupled thermo-mechanical FE model was developed to identify MIS values as the results of multi-scanning laser paths in the mesoscale model. Temperature-dependent material properties were defined to enhance the accuracy of the simulation. Initially, a comprehensive thermal analysis was conducted for the specified geometry and boundary conditions, followed by applying the resulting temperature histories as the thermal load in the mechanical analysis. Custom Python scripts and user subroutines were developed to extend Abaqus capabilities and equip it with essential tools for enhancing the accuracy of the non-linear thermo-mechanical simulation. An agglomeration (layer-lumping) approach was formulated to transfer an equivalent MIS field from the mesoscale model to the macroscale model. In this technique at the macroscale level, many physical powder layers were lumped into one larger equivalent computational layer, and the governing mechanical system of equations was solved. Experimental studies on printed cantilever beams were also conducted to validate the predicted residual stress and distortion using the developed FE model for Inconel-718. Among four common

material plasticity behaviors, including EPP, IsoH, KinH, and JC, the KinH model could achieve the best prediction accuracy with smaller number of equivalent layers. This result revealed the importance of material constitute models including realistic hardening behavior to enhance the accuracy of the prediction in the MIS method for complex parts. Results also suggested that in-plane anisotropic stresses are the primary cause of part distortion due to the formation of residual stresses on the near surface layers.

Additionally, a systematic investigation was conducted on the MIS-based residual stress predictions against depth-resolved XRD measurements in the subsurface for cube coupons fabricated by Inconel-625. It was found that while the experimentally validated MIS-based model can predict the near surface residual stresses with high accuracy, it underestimates tensile residual stresses beyond 1 mm depth, failing to capture the experimental XRD stress peak. This discrepancy, driven by simplified thermal-mechanical coupling and uniform plastic strain assumptions, highlights its limits for subsurface stress prediction in multi-layer LPBF builds. Findings also highlighted that residual stress rises with increasing laser power but drops at higher levels due to keyhole effects, revealing a non-monotonic trend. In addition, increasing scanning speed effectively lowers residual stresses, emphasizing its dominant role in thermal gradient and stress control.

Finally, a hybrid FE-ML coupled model was developed to accelerate the prediction of residual stresses and distortions in the multi-scale MIS model. The study was undertaken to investigate the applicability and implementation of data-driven analysis for the MIS predictions in the mesoscale simulation. By incorporating the comprehensive influence of processing parameters for three widely used nickel-based superalloys, along with the effects of heat source characteristics, nodal temperature, and nodal coordinates, the research underscored both the novelty and practical significance of this approach for rapid and efficient stress and distortion prediction. Five ML algorithms were evaluated for MIS prediction using simulation-derived data. Among these, CatBoost, KNN, and optimized KNN demonstrated superior predictive performance for IS in the longitudinal, transverse, and layer-thickness directions. Experimental validation through cantilever beam distortion confirmed the robustness and reliability of the models. Overall, the developed hybrid FE-ML model achieved up to a 10,000-fold reduction in computational time compared to conventional multi-scale FE simulations.

Collectively, these results demonstrate that incorporating realistic hardening behavior within MIS-based frameworks is essential for accurate residual stress prediction in LPBF, that current MIS formulations require refinement for reliable subsurface stress estimation, and that hybrid FE–ML strategies can make high-fidelity process simulation practically usable at the part scale. These advances provide a concrete pathway toward more predictive and computationally viable LPBF process design tools.

6.2 Contributions

The main contributions of this research can be summarized as follows:

- As part of this research, a comprehensive review article was published in a high-impact, peer-reviewed journal to critically evaluate the current state of knowledge in the field of LPBF process modeling and residual stress prediction by IS method. This review systematically examined recent advances, key challenges, and emerging trends in IS numerical methodology, providing an integrated framework for understanding the thermo-mechanical approaches, the multi-scale mechanisms governing IS evolution, thermal gradients, distortion formation, and process parameter optimization. By consolidating over 90 peer-reviewed studies and highlighting gaps in predictive modeling and data-driven approaches, the paper established a solid conceptual and methodological foundation for the subsequent investigations presented in this thesis. The publication has received considerable recognition within the research community so far, which underscores its relevance and impact in advancing the current understanding of the topic.
- Another key contribution of this research involved a comprehensive investigation into the influence of hardening behavior and material plasticity models on the accuracy of LPBF process simulations within the MIS framework. This study addressed a significant gap in the existing literature, where most prior works have simplified material behavior by assuming an idealized elastic–perfectly plastic response for computational convenience. Through a detailed comparative analysis of different hardening models, the results revealed that the KinH model provides a more realistic and reliable representation of the material’s cyclic plasticity and strain evolution during the LPBF process. The findings underscore the necessity of incorporating advanced hardening laws in thermo-mechanical simulations to enhance the predictive fidelity of residual stress and distortion analyses.

- This research also makes a significant contribution to the understanding of residual stress formation within the IS-based or MIS-based modeling frameworks by providing a depth-resolved experimental validation that has not been previously reported in the literature. Specifically, the MIS-based residual stress prediction was systematically validated against depth-dependent XRD measurements obtained along the longitudinal, transverse, and build directions at incremental depths of 0 μm , 1000 μm , 2000 μm , and 3000 μm . This comprehensive validation approach enabled a direct comparison between simulated and experimentally measured stress profiles, thereby establishing the accuracy and robustness of the MIS methodology in capturing the subsurface stress gradients inherent to the LPBF process. The findings offer novel insights into the three-dimensional evolution of residual stresses beneath the surface of additively manufactured components and effectively bridge a critical gap in current LPBF modeling research.
- In the context of data-driven modeling for residual stress and distortion prediction in LPBF, most existing studies have focused on a limited subset of processing or material parameters. The present research advances the state of the art by developing a comprehensive data-driven framework that captures the combined influence of all critical factors governing the MIS behavior. These factors include key process parameters such as laser power, scanning speed, layer thickness, hatching space, and scanning strategy, along with supplementary variables such as heat source characteristics, material properties, nodal temperature histories, nodal depth coordinate, and the number of microscale layers. By integrating these multidimensional inputs, the proposed approach enables the rapid and accurate prediction of IS components across different build conditions. Furthermore, this study systematically evaluated and identified the ML algorithms exhibiting the highest predictive performance for small and complex datasets, thereby establishing an efficient and reliable methodology for IS prediction in multi-scale LPBF simulations and process parameter optimization.

6.3 Future works

This research has contributed significantly to advancing the understanding of the complex physical phenomena and modeling challenges associated with LPBF through the integration of both numerical and data-driven approaches. Despite the substantial progress achieved, the inherently non-linear and multi-physics nature of the LPBF process presents continued challenges that leaves avenues for further investigation. Building on the findings of the present study, the following

directions are proposed to enhance the predictive accuracy, computational efficiency, and practical applicability of LPBF process modeling.

- Incorporating transient thermal cycling more explicitly into the MIS method to improve the accuracy of the subsurface stress predictions. This can be achieved by integrating adaptive strain calibration based on layer-specific thermal histories in the macroscale simulation.
- Extend the developed hybrid FE-ML model to lattice structures and highly complex geometries, thereby supporting the most demanding additive manufacturing designs and assessing model performance under extreme geometrical and loading conditions.
- The developed hybrid FE–ML model significantly reduced the computational time required for the IS calculation and subsequent macroscale residual stress and distortion predictions. However, future work could focus on enhancing training efficiency through GPU-accelerated computation and parallelized learning techniques, enabling faster and more scalable model implementation.
- Incorporating ML algorithms to predict the melt pool dimensions across a wide range of material types. This framework allows for the efficient generation of extensive datasets required for IS prediction, significantly reducing reliance on resource-intensive experimental procedures, facilitating the process parameter optimization.
- Developing digital twin frameworks, potentially leveraging physics-informed neural networks (PINNs) to predict inherent strains without relying on thermal simulations, thereby advancing toward real-time process monitoring, control, and optimization.

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