

Tailoring residual stress in wire-based directed energy deposition of ferritic steel through experiments and AI driven thermo-mechanical model

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Tailoring residual stress in wire-based directed energy deposition of ferritic steel through experiments and AI driven thermo-mechanical model

A thesis submitted in partial fulfilment for the award of the degree of

Doctor of Philosophy

by

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2026



Dedicated to

Lord Hanuman-Shri Ram, Parent, Sister,
Teacher, and my wife



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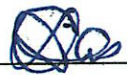
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CERTIFICATE

It is certified that the work contained in the thesis entitled “*Tailoring residual stress in wire based directed energy deposition of ferritic steel through experiments and AI driven thermo-mechanical model*” submitted by **Mr. Amritesh Kumar** to the Indian Institute of Technology Guwahati for the award of the degree of doctor of Philosophy has been carried out under our supervision in the Department of Mechanical Engineering, Indian Institute of Technology Guwahati. This work has not been submitted elsewhere for the award of any other degree or diploma.

The thesis, in my opinion, has reached the standard fulfilling the requirements for the award of degree of Doctor of Philosophy in accordance with the regulations of the Institute.

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Declaration

I declare that the present written submission is my thoughts in my own words. I have adequately been cited and referenced the original sources, where others' ideas have been involved. I also declare that I have followed all principles of academic morality and honesty and have neither fabricated nor falsified any idea/data in the present thesis. I realize that any defilement of the above will be cause for disciplinary action by the Institute and can also induce disciplinary action from the sources which have thus not been properly cited.

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ABSTRACT

Residual stress evolution critically governs the structural integrity and performance of thin walls fabricated by wire-based directed energy deposition (DED) process. This study presents an integrated experimental-computational-artificial intelligence (AI) framework to tailor residual stresses in 9Cr-1Mo steel deposits. Thin-wall and multi-track multi-layer structures are fabricated by employing cold metal transfer (CMT) based deposition at diverse scanning strategies, with in-situ thermocouple measurements and XRD-based residual stress evaluation. Microstructural and mechanical characterizations revealed the presence of a lath martensitic matrix with δ -ferrite and uniformly distributed carbides ($M_{23}C_6$, MX), which contributed to strengthening. Fractography indicated a transition from quasi-cleavage to ductile fracture with bi-directional scanning, accompanied by improvements in tensile strength and enhanced structural performance. A finite element (FE)-based thermal-metallurgical-mechanical (TMM) model computes the residual stress incorporating the effect of volumetric strain due to martensitic transformation. The study depicts that tensile stresses increase sharply with prolonged inter-layer dwell times, whereas optimized dwell-time and scanning strategies (spiral-in, bi-directional, and mixed patterns) promoted uniform heat dissipation that leads to reduction in residual stresses. The critical role of linear energy density in mitigating stresses and distortions along the build height is also established. Complementing physics-based modeling, physics-informed deep learning (PIDL) surrogates are trained by FE results and experimental datasets. Temporal convolutional networks (TCN) exhibited the highest fidelity in predicting transient residual stress evolution. PIDL models further enabled inverse design by accurately estimating deposition attributes such as power, velocity, and dwell time for targeted thermal or stress thresholds, demonstrating robust predictive performance even in extrapolation regimes. Additionally, TCN models accurately predict the dilatometry curve for unknown advanced scanning patterns enabling improved stress estimation within the coupled TMM framework. Overall, this study establishes an integrated framework that combines experiments, FE-based TMM simulations, and AI surrogates to intelligently design deposition strategies. The results reveal that careful modulation of inter-layer dwell time, energy density, and scanning strategies can significantly reduce tensile residual stresses and enhance the structural and mechanical performance of wire-arc additively manufactured 9Cr-1Mo steel.

Keywords: Additive manufacturing, Wire-based DED, cold metal transfer, residual stress, phase transformation, finite element modeling, artificial intelligence, deep learning, ferritic–martensitic steels.

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List of acronyms

Acronyms	Description
AM	Additive manufacturing
MAM	Metal additive manufacturing
DDM	Direct digital manufacturing
3DP	Three-dimensional printing
SFF	Solid freeform fabrication
RP	Rapid prototyping
DED	Directed energy deposition process
WAAM	Wire arc additive manufacturing
GMAW	Gas metal arc welding
CMT	Cold metal transfer
PAW	Plasma arc welding
PBF	Powder bed fusion
AUSC	Advanced ultra-supercritical power plants
CSEF	Creep strength enhanced ferritic steel
MEAs	Medium-entropy alloys
EDM	Electrical discharge machining
HAZ	Heat affected zone
LPBF	Laser powder bed fusion
XRD	X-ray diffraction
EDX	Energy dispersive X-ray
EBSD	Electron backscatter diffraction
KAM	Kernel average misorientation
IQ	Image quality maps
GOS	grain orientation spread maps
IPF	Inverse pole figure
TEM	Transmission electron microscopy
SEM	Scanning electron microscopy
FCC	Face-centred cubic
BCT	Body-centred tetragonal
UTS	Ultimate tensile strength
YS	Yield strength
DOF	Degree of freedom

FEM	Finite element method
TMM	Thermal-metallurgical-mechanical
MT	Martensitic transformation
TRIP	Transformation-induced plasticity
KM	Koistinen–Marburger
IHPP	Inverse heat placement problem
ML	Machine learning
PIML	Physics-informed machine learning
DL	Deep learning
PIDL	Physics-informed deep learning
RNN	Recurrent neural networks
DNN	Deep neural networks
AI	Artificial intelligence
DT	Decision tree
ERT	Extremely randomized tree
RF	Random forest
KNN	K-nearest neighbours
SVR	Support vector regressor
XGBOOST	Extreme gradient boosting
ANN	Artificial neural network
MLPs	Multilayer perceptron's
LSTM	Long short-term memory
Bi-LSTM	Bidirectional long short-term memory
GRU	Gated recurrent unit
TCN	Temporal convolution neural network
RMSE	Root means square error
ReLU	Rectified linear unit

Nomenclature

Symbol	Description	Unit
d	Inter-planar spacing	Å
k	Thermal conductivity	$\text{W m}^{-1}\text{K}^{-1}$
V	Deposition speed	mm s^{-1}
θ	Bragg angle	degree
ν	Poisson ratio	-
Ψ	Polar angles to the tensor coordinate system	-
t	Time	s
a_f	Extent of heat source from its center in the front ellipsoid	-
a_r	Extent of heat source from its center in the rear ellipsoid	-
f_f	Heat distribution in front part of ellipsoid	-
f_r	Heat distribution in rear part of ellipsoid	-
q_f	Heat flux in front part of ellipsoid	W m^{-2}
q_r	Heat flux in rear part of ellipsoid	W m^{-2}
ε	Elastic strain	-
δ_{ij}	Kronecker delta	-
$\Delta\varepsilon_{ij}^{total}$	Total incremental strain	-
$\Delta\varepsilon_{ij}^e$	Elastic strain	-
$\Delta\varepsilon_{ij}^{th}$	Thermal strain	-
$\Delta\varepsilon_{ij}^p$	Plastic strain	-
$\Delta\varepsilon_{ij}^v$	Volumetric strain	-
$\Delta\varepsilon_{lm}^{th}$	Thermal strain	-
α	Coefficient of thermal expansion	$^{\circ}\text{C}^{-1}$
T_0	Initial temperature	$^{\circ}\text{C}$
A_{c1}	Austenitic start temperature	$^{\circ}\text{C}$
A_{c3}	Austenitic finish temperature	$^{\circ}\text{C}$
M_s	Martensitic start temperature	$^{\circ}\text{C}$
M_f	Martensitic finish temperature	$^{\circ}\text{C}$
C	Stiffness matrix of fourth order	MPa
D_{ijlm}	Elastic stiffness matrix	MPa
ΔT	Temperature difference	$^{\circ}\text{C}$
F_A	Fraction of austenite	-
F_M	Fraction of martensite	-

k	Koistinen–Marburger (K–M) constant	$^{\circ}\text{C}^{-1}$
T_{sa}	Threshold temperature for the M→A transformation	$^{\circ}\text{C}$
$\dot{Q}$	Heat generation rate per unit volume	J/mm^3
K_m	Kinetic-mechanical index	$^{\circ}\text{C}^{-1}$
R^2	Coefficient of determination	-
RMSE	Root means square error	-
dh_m	Transformation enthalpy	Jm^{-3}
$\Delta\varepsilon_{ptm}$	Volumetric transformation-induced strain	-



Chapter 1

Introduction

1.1 General background

Metal-based additive manufacturing (AM) has revolutionized the production of high-performance components through its ability to fabricate complex geometries directly from digital models. By depositing material in a layer-by-layer manner, AM eliminates many of the geometric and processing constraints associated with traditional subtractive manufacturing. It enables design freedom, material efficiency, and reduced lead times, making it particularly attractive for aerospace, automotive, biomedical, and energy sectors [1,2]. Among various terminologies used to describe this technology such as three-dimensional printing (3DP), rapid prototyping (RP), direct digital manufacturing (DDM), and solid freeform fabrication (SFF), additive manufacturing (AM) has become a cornerstone of modern manufacturing innovation. According to ASTM standard F2792-12a, metal AM technologies are broadly categorized into powder bed fusion (PBF) and directed energy deposition (DED), based on how feedstock material is delivered and fused [1]. In a DED based AM process, the fabrication of a component is performed by melting of feedstock materials (wire, powder, or sheet) using a suitable heat source (laser, electric arc, or electron beam). Within this category, cold metal transfer (CMT) based DED has garnered increasing attention due to its low heat input, high deposition rates, and minimal spatter, which collectively contribute to better control over microstructure and mechanical properties.

9Cr-1Mo steel, a creep strength-enhanced ferritic (CSEF) alloy, exhibits excellent creep-rupture properties and high corrosion resistance under extreme conditions (temperature $>750^{\circ}\text{C}$ and pressure $>27.5\text{ MPa}$) [3]. These attributes make it the preferred material for critical

components such as headers and tubes in boilers for advanced ultra-supercritical (AUSC) power plants [4]. However, conventional fabrication methods for such components are time-intensive, prompting interest in AM techniques, particularly DED. Despite its potential, the adoption of AM for 9Cr-1Mo steel remains limited due to the challenges associated with rapid heating/cooling cycles, which result in microstructural heterogeneity, anisotropic mechanical properties, and residual stress accumulation [5]. Wire arc additive manufacturing (WAAM) process has received significant attention because of its potential to manufacture large and complex parts with less production cost [6]. The deposition attributes are also controlled by different levels of heat input and deposition strategy in a WAAM process [7]. On deposition, the kinetics and dynamics of the molten pool is influenced by scanning strategies [8,9]. The re-melting and solidification of deposits takes place in a cyclic manner that leads to the non-uniform expansion and contraction of deposited material. Hence, the variation of microstructure and resulting residual stress formation are direct consequences associated with heat input strategy. All these physical phenomena are directly correlated with non-uniform distribution of temperature profiles often detected by molten pool dynamics of the deposited layer. Materials like CSEF steels, especially 9-Cr-1Mo, are more sensitive to temperature changes that lead to microstructural change and development of inter-locked stresses. Moreover, during arc DED process, the material is subjected to rapid heating and cooling cycles, leading to solid-state austenite-to-martensite transformation accompanied by a volumetric expansion [1,10]. While this transformation contributes to strength enhancement, it also induces substantial tensile residual stresses due to constrained thermal contraction during cooling. These stresses can compromise the structural reliability of components, particularly in the heat-affected zone, where they facilitate localized creep damage and premature failure commonly referred to as Type IV cracking [3]. Such cracking is especially critical in manufacturing components of layer-by-layer deposition process, where mechanical integrity is vital over prolonged high-temperature exposure. As a result, understanding the thermal and phase transformation history during deposition is essential to minimize stress accumulation and ensure dimensional accuracy and mechanical performance of 9Cr-1Mo steel builds.

1.2 Current Status

Gas metal arc welding (GMAW) and CMT are widely used variants of the WAAM process due to their distinct metal transfer characteristics. GMAW-based metal transfer is advantageous for fabricating large-scale components because of its high deposition rates achieved at relatively high heat input [11]. However, this process exhibits limitations, such as instability of the arc and an enlarged molten pool size, which adversely affect the quality of the printed surface and restrict the minimum achievable thickness of the manufactured parts [6]. Although extensively studied, the literature often lacks detailed insights into the effects of arc instability and molten pool dynamics on microstructure formation and defect evolution in GMAW-based WAAM, particularly for high-strength materials. On the other hand, the CMT-based WAAM process, with its exceptionally stable arc, minimal spattering, and precisely controlled thermal input, facilitates smooth metal transfer [8,12]. The higher cooling rates achieved in CMT (nearly double those in GMAW) result in refined grain structure and enhanced mechanical properties in printed components [13,14]. Despite these advantages, a gap remains in understanding how specific thermal cycles and cooling rates in CMT-based WAAM influence phase transformations and anisotropic mechanical behavior in different materials. CMT-based WAAM has emerged as a promising technique for fabricating a wide range of materials, including aluminum [15,16], magnesium [17], steels [18,19], titanium [20,21], and nickel-based superalloys [22]. However, the existing literature is largely observational, with limited focus on material-specific thermal gradients, microstructural evolution, and residual stress formation. For instance, aluminum and magnesium alloys, while widely studied, exhibit distinct challenges such as susceptibility to cracking and oxidation, yet there is a lack of systematic investigations into optimizing CMT process parameters to mitigate these issues. Similarly, for high-performance alloys like nickel-based superalloys, studies predominantly report experimental outcomes without critically analyzing the long-term stability of the microstructure under service conditions.

Post-processing treatments are a widely recognized methodology for enhancing the performance of AM-fabricated components. Homogenization at 1200°C and aging at 760°C significantly improve the properties of plasma arc welding (PAW)-based DED components [22], whereas superior performance of laser-based DED of steels is achieved by precise control over heat input [23]. Mukherjee et al. [10] provided insights into optimizing thermal cycles

using tempering kinetics of steels. The normalization followed by tempering has been shown to enhance the ductility of 9Cr-1Mo steel by dissolving precipitates [23]. However, confidence on post-processing poses challenges for components with complex geometries, such as headers and tubes in AUSC power plants. In addition, layer-by-layer deposition of dissimilar P91 steel and Inconel 740H suffer from residual stress and strain localization issues [26], emphasizing the need for precise thermal management during fabrication. Similarly, Billingham et al. [24] proposed solving the inverse heat placement problem (IHPP) as a method for achieving uniform temperature distribution. However, the practical implication of the same is still challenging. This insightful understanding shows the importance of advanced in-process system development than a conventional post-processing system.

In arc based DED process, any perturbation in deposition process experiences an abrupt change in temperature distribution. During the solidification of the molten pool, it may experience several defects like gas entrapment, lack of fusion, and solidification cracking [1-2]. The phase transformation leads to microstructural changes and the evolution of type –II residual stress due to spatial variation of temperature gradients during cooling of molten material [1]. The analysis of thermal behavior, such as the accumulation of heat and its variation with different deposition parameters, plays a significant role in making a defect-free component with high degree of functionality. Although experimental techniques are more insightful, their latitudes are very limited. For example, once a layer is stacked on already printed part, the measurement of temperature or stress at that layer is cumbersome or almost impossible. Heat input to create the molten pool directly affects printability of the DED fabricated parts that are highly correlated with the deposition parameters. Relatively high heat input of a moving arc at any momentary location leads to dynamicity of depositing liquid metal that in turn affect the solidification behavior and evolution of inter-locked stresses [25]. When a substantially higher magnitude of residual stress evolves in the final component, it may lead to the formation of cracks and deteriorate the mechanical properties. However, the induced residual stress can be mitigated by optimizing the DED attributes and scanning strategies [7]. Several experimental studies have been performed to find out the intrinsic relationship between deposition attributes (heat input, layer thickness, inter-layer dwell times, deposition strategy, substrate thickness, deposition height, inter-layer temperature) [26–30], and their microstructural-mechanical characteristics [31]. It is evident that several non-linear relations

exist between input and output parameters to comply with the optimum set of parameters in an AM component. However, the establishment of non-linear relations demands huge experimental data. For unravelling these barriers, the development of a computational model in the context of large input process parameters-based AM technique facilitates to tackle the issues quite efficiently for a thin-wall printed structure.

A physics-based numerical model of the WAAM process facilitates a phenomenological understanding of the effect of DED parameters on the thermal-metallurgical-mechanical performance of a printed component. The physical elements of WAAM process consists of filler wire melting, formation of droplets, transportation of droplets, flow behavior of molten metal, and various modes of heat transfer [32]. Implementing all these physiognomies in a single model for the computation of residual stress is a tedious task. Moreover, measurement of temperature by infrared camera for a movable object and multi-deposited tracks on the liquid molten pool is cumbersome or almost impossible [3,4]. The thermocouple measures temperature by a contact method, but it is associated with a response time lag. Hence, in-situ monitoring of the rapid melting and cooling is not always possible with available measurement techniques. To evaluate the temperature in AM deposits, a physics-based model (analytical and numerical) is more appropriately used [33,34]. It requires solving of mass, momentum, and energy conservation equations with suitable boundary condition. The solution of 3D flow field is computationally intensive. Hence, the finite element (FE) based numerical simulation of DED processes is utilized to elucidate only the thermo-mechanical responses of the fabricated components [35–41]. To date, developing a well-tested and computationally efficient model for predicting residual stress and distortion in AM process is a challenging task [42,43].

Depending on the model characteristics such as geometrical features, material properties, boundary conditions, and complexity of the problem, the computational time of the simulation varies from minutes to several hours or even days to complete the analysis. This drives us to realize that there is a requirement for the development of an efficient tool for in-situ monitoring and control of complex physical phenomena and decision-making routes for the AM industry. All of this can be achieved by not only a highly accurate physical process model but also integration with data-driven models [44–47]. The choice of a proper data-driven model with physical features from a phenomenological process model is usually termed as physics-

informed deep learning (PIDL) model that dictates the computational efficiency of the integrated algorithm and practical applicability of the DED process [48–50]. Implementation of DL models have been recently explored as these techniques have proven capability of confining the nonlinear correlations between input and output features [51–57]. The DL models such as artificial neural network (ANN), convolutional neural network (CNN), and recurrent neural network (RNN) have been widely used as pure data-driven models for enhancing the quality of printed parts [58–61].

It is observed that PIDL framework is utilized to predict 3D temperature distribution for laser based metal deposition process with approximately 2% error and considerably savings of the computational time as compared to only FE model [62]. Ren et al. [63] used RNN model to elucidate the thermal behavior of multi-track deposition process in a physics-based machine learning module. However, the computational time is significant for more than a single layer of deposition. The limitation of this study is overwhelmed by implementing temporal convolutional network (TCN) type DL models, which require less training time compared to other ANN models [31]. However, the physical phenomena is imparted to this TCN model from an experimentally validated FE model. A similar approach is followed with reasonable accuracy for in-situ monitoring of the dimension of the molten pool and evolved transient thermal profile in cold metal transfer-based DED process [41]. Ness et al. [64] developed data-driven framework for predicting the temperature profiles of arc-based DED process by extremely randomized tree (ERT) regression model. The model is trained by using physics-based features pertaining to the scanning strategy for the prediction of transient thermal profiles. In various studies, the thermal histories for different geometrical features and consequently developed residual stress is predicted by the ANN models [65,66]. It is realized that the algorithms developed by integrating FE and ANN model facilitates computationally efficient approach and enhances the prediction capability of residual stress distribution for an intricate part. The role of DL models is quite successful to forge a link between the input parameters and its corresponding impact for an AM part.

When a large number of deposition variables are correlated to each other in a non-linear fashion, it is quite difficult to identify such co-relation and their combined effect on a printed component. Hence, ML algorithms have the unique capabilities of getting useful insights from the data given for training and providing the correlation between input features and output

variables [67]. Few of the ML algorithms like extreme gradient boosting (XGBOOST), Random forest (RF), and artificial neural network (ANN) models fit well with non-linear datasets and can provide relatively accurate predictions without any prior knowledge of physics applied for generating such data in AM processes [68–70]. The application of ML algorithms in the AM sector is limited because large number of experimental data is required for training and interpretation of the same as feature. Even the data that have physical significance consists of a number of pre-processing steps to create a complete dataset [71]. A well-tested FE model is a good source for generating data for ML models for a large number of process variables. PIML model (combined FE and ML) has been reported in the existing literature for analyzing different deposition attributes on additively manufactured components [63,72,73]. Hajjalizadeh et al. [72] developed an ANN model integrated with the FE model for the computation of residual stresses in different deposited structures. The transient temperature evolution for multi-layer deposition with varying heat input levels for a WAAM process is analyzed by ANN [74]. Mukherjee et al. [69] predicted the maximum longitudinal residual stress of a deposit by ANN and RF models, and FE model. Ren et al. [63] conducted a combined study of the FE model and recurrent neural networks and deep neural networks (RNN-DNN) at different scanning strategies. However, most of the reported work in AM technologies is aligned to predict single data points as compared to complete non-linear profiles by ML algorithms.

1.3 Significance of present study

The discussion in literature illustrates the fact that arc-based DED processes are significantly replacing conventional manufacturing methods for fabricating critical structural components. Numerous studies are currently underway to enable the additive manufacturing of geometrically complex and mechanically robust parts. Components such as thermowells, which are designed to operate under extreme thermal and mechanical conditions, demand high-quality printing with tailored microstructural evolution to ensure optimal performance and durability. Achieving such precision in microstructure requires a deep understanding and control of the thermal history during deposition, as it directly governs phase transformation and residual stress development. In this context, 9Cr-1Mo steel has emerged as a widely used material in power plants, pressure vessels, and high-temperature AUSC applications due to its

excellent creep resistance, thermal stability, and mechanical strength. However, it remains highly sensitive to thermal gradients and phase transformations, especially in the heat-affected zone (HAZ), which makes it susceptible to Type IV creep failure. Conventional manufacturing approaches struggle to mitigate these challenges effectively. AM process using arc-based DED provides a viable alternative by enabling high deposition rate and localized microstructural control, provided that thermal management is optimized. Among various arc-based deposition techniques, the CMT process offers distinct advantages for 9Cr-1Mo steel due to its low heat input, stable arc characteristics, and spatter-free deposition, which collectively facilitate refined microstructure and reduce thermal distortion. These benefits make CMT-based DED particularly suitable for building ferritic-martensitic components where microstructural integrity and residual stress control are paramount.

In the current study, an in-process optimization of the CMT-based DED process is targeted to address the critical challenges associated with residual stress management and microstructural control in 9Cr-1Mo steel. Bi-directional scanning strategies are introduced as an effective means to reduce localized heat accumulation, minimize sharp thermal gradients, and promote more uniform temperature distribution during deposition. These strategies significantly mitigate residual stress, which is a key contributor to Type IV cracking observed under high-temperature creep conditions. By ensuring consistent cooling rates along the build direction, bi-directional scanning facilitates stable microstructural evolution, aiding in the uniform precipitation of strengthening phases such as $M_{23}C_6$ and MX carbides. This enhances inter-layer cohesion and mechanical reliability in the as-built structure. To deepen the understanding of these complex interactions, thermodynamic modeling is employed to analyze key phase transformations such as martensite stabilization and δ -ferrite dissolution under non-equilibrium conditions typical of DED. FE based thermo-mechanical simulations capture the interplay between heat input, cooling rate, and residual stress, providing a predictive platform for optimizing deposition strategies. Experimental validation is carried out using EBSD, including Kernel Average Misorientation (KAM) mapping and phase fraction analysis, to confirm simulation-predicted microstructural evolution. Results demonstrate that bi-directional scanning not only refines martensitic laths but also reduces dislocation tangles, contributing to enhanced mechanical performance and creep resistance.

To further enhance the printability of 9Cr-1Mo steel component this study introduces a segmented strategy that couples scan path engineering with control over martensitic transformation and residual stress evolution. Six scanning strategies, namely longitudinal, transverse, spiral-in, spiral-out, inclined, and circular are systematically evaluated using thermo-metallurgical-mechanical model. Based on insights from thermal gradients and stress fields, unique S-pattern and mixed-path strategies are proposed to spatially modulate martensitic transformation and reduce tensile residual stress. These strategies exploit localized thermal gradients to control transformation kinetics and spatial martensite distribution. The effectiveness of the proposed methods is validated through comprehensive experimental characterization, including X-ray diffraction (XRD)-based residual stress measurements, electron backscatter diffraction (EBSD) analysis, and dilatometry. These analyses confirm strong correlations among thermal history, phase transformation behavior, and residual stress development.

A FE-based thermo-metallurgical-mechanical model is essential for capturing the complex physical interactions occurring during the arc-based DED of 9Cr-1Mo steel. This steel grade is widely used in high-temperature applications due to its excellent creep resistance and strength, but it is also highly sensitive to thermal gradients and transformation-induced plasticity. The layer-by-layer thermal cycling inherent in the DED process causes rapid heating and cooling, leading to phase transformations such as the formation of martensite, which in turn influences residual stress development. The FE model, by incorporating temperature-dependent material properties and transformation strain effects, enables accurate computation of the thermal field, prediction of phase transformation kinetics, and evaluation of residual stress evolution throughout the build. However, while accurate, this high-fidelity modeling is computationally expensive and not suitable for real-time or in-situ process control. To address this limitation, machine learning (ML) models such as RF, Decision Tree (DT), K-Nearest Neighbors (KNN), Support Vector Regression (SVR), and ANN are introduced as data-driven alternatives for predicting transient thermal profiles. These models are trained on a large dataset generated from validated FE simulations, enabling them to capture the relationships between input process parameters (e.g., power, velocity, time) and temperature evolution. Once trained, these ML models can offer rapid predictions at a fraction of the computational cost, making them highly suitable for in-situ monitoring and process feedback control. This

integration of ML with numerical simulation forms the basis for real-time thermal regulation, which is critical for maintaining thermal stability and controlling phase transformation during the printing process. Building upon this, ANNs are further leveraged to predict not just thermal profiles but also the residual stress distribution along the build height under various inter-layer dwell times. Since dwell time directly affects the inter-pass temperature and cooling rate, it plays a crucial role in determining thermal gradients and stress development. ANNs, with their ability to model complex non-linear dependencies, are well-suited to predict how variations in dwell time influence the resulting temperature and stress fields. This capability allows for rapid evaluation of multiple deposition scenarios, enabling intelligent process planning without resorting to repeated FE simulations.

To enhance this forward prediction capability, the study also explores inverse modeling approach to determine optimal inter-layer dwell times that yield desired thermal or residual stress outcomes. Instead of simply predicting the effects of dwell time, the inverse approach enables the model to suggest appropriate dwell durations that minimize residual stress accumulation and promote microstructural uniformity. This is particularly valuable for adaptive control in layer-by-layer fabrication, where local adjustment of dwell times can significantly improve print quality and mitigate issues such as Type IV cracking or poor inter-layer bonding. While residual stress and thermal fields are critical, understanding transformation-induced strain is equally important for comprehensive stress modeling. To this end, the study incorporates temporal convolutional Networks (TCNs) to predict dilatometric strain from transient thermal histories. Unlike traditional feedforward networks, TCNs are designed for time-series data and can effectively capture the temporal dynamics of phase transformations such as the martensitic transformation in 9Cr-1Mo steel. Trained on experimental dilatometry datasets, the TCN model provides fast and accurate predictions of transformation strain, which can then be integrated into the FE or ANN-based stress models for improved fidelity. This hybrid approach of combining deep learning with physics-based modeling ensures a holistic understanding of the thermo-metallurgical-mechanical behavior of the printed part. In summary, the synergy between high-fidelity FE simulations and intelligent machine learning models forms a powerful framework for predictive and adaptive control of the DED process. By linking thermal profiles, phase transformations, residual stresses, and dilatometric strain, the study not only advances the scientific understanding of additive

manufacturing of 9Cr-1Mo steel but also provides practical tools for improving build quality, process efficiency, and long-term structural integrity in high-temperature applications.

1.4 Problem statement

To summarize the current work, deposition characteristics of 9Cr-1Mo steel is investigated into three verticals consists of experimental characterization, numerical simulation, and artificial intelligence (AI)-based modelling to provide a holistic understanding and control of AM process for high-performance components. In the first vertical, an extensive suite of experimental characterization techniques is employed to examine the bead characteristics, microstructural evolution and mechanical behaviour of the deposited 9Cr-1Mo steel. Microstructural features such as martensitic grain morphology, sub-grain structures, phase distribution and precipitates analysis are studied using optical microscopy, scanning electron microscopy (SEM), and electron backscatter diffraction (EBSD). EBSD maps provide detailed insights into grain orientation, Kernel Average Misorientation (KAM), grain boundary character, and phase fractions, helping to decode the microstructural evolution in fabricated part printed using different scan strategies. Residual stress distributions are experimentally quantified using X-ray diffraction (XRD), while phase transformation behaviour is assessed through dilatometric analysis. Mechanical properties are evaluated using standardized microhardness and tensile testing in accordance with ASTM standard confirming the structural soundness and performance of the builds under various thermal histories. This experimental vertical validates the influence of bi-directional and engineered scan strategies on martensitic refinement, dislocation evolution, carbide precipitation ($M_{23}C_6$ and MX), and inter-layer bonding, providing essential feedback for model calibration and training.

The second vertical is anchored on a FE-based thermo-metallurgical-mechanical (TMM) model is developed to simulate the complex interactions occurring during CMT based DED process of 9Cr-1Mo steel. This comprehensive framework captures the interdependent effects of heat transfer, phase transformation, and mechanical response under non-equilibrium processing conditions. The thermal module computes the transient temperature distribution during the layer-by-layer deposition, accounting for moving heat sources, deposition sequence, and interlayer dwell times. The metallurgical module integrates thermodynamic and kinetic models to predict phase transformations such as austenite formation, δ -ferrite dissolution, and

martensitic transformation, as well as the precipitation behaviour of secondary phases like $M_{23}C_6$ and MX carbides. The mechanical module calculates the evolution of stress and strain fields, incorporating thermal expansion, transformation-induced plasticity (TRIP), and phase transformation strains. This coupled modelling approach provides a high-fidelity representation of the DED process, enabling the prediction of residual stress accumulation, distortion, and microstructural gradients. By linking thermal history with metallurgical phase evolution and mechanical deformation, the model serves as a powerful tool for process optimization and component integrity assessment. It also generates the data foundation for training machine learning algorithms, ensuring that data-driven predictions are physically informed and experimentally validated.

The third vertical introduces a hybrid artificial intelligence framework to accelerate and augment the predictive capability of the study. In this approach, deep learning models, particularly TCNs are employed to predict dilatometric strain and residual stress evolution based on simulated and experimental thermal histories. The models are trained using a dataset generated from physics-based simulations and validated by experimental dilatometry, providing high-fidelity predictions of martensitic transformation behaviour under varying process conditions. Additionally, physics-informed machine learning (PIML) models are implemented to estimate both transient temperature profiles (multi-point outputs) and peak temperature (single-point output) for a wide range of input process parameters, including arc power and deposition velocity. The process window consists of 121 numerically simulated cases, each contributing to the development of a surrogate model capable of bypassing expensive simulations for real-time decision-making. Five machine learning algorithms with varying nonlinear capabilities are benchmarked, and the models demonstrating the highest accuracy are used for predictive tasks. Furthermore, the AI framework is extended to assess the influence of inter-layer dwell time on residual stress evolution by correlating non-linear thermal profiles with stress distributions. This coupling of data-driven models with experimentally validated simulations creates a fast, scalable, and physically consistent platform for residual stress prediction.

This integrated, tri-axial approach not only enhances the scientific understanding of how thermal history and scanning strategy influence microstructural evolution and residual stress development in 9Cr-1Mo steel but also provides a practical roadmap for optimizing arc-based

DED processes. The study contributes a novel scan-path engineering methodology that mitigates Type IV creep-prone zones through controlled martensitic transformation and localized stress relaxation. The development and validation of unique S-pattern and mixed scan strategies informed by six conventional patterns (longitudinal, transverse, spiral-in, spiral-out, inclined, and circular) demonstrate the effectiveness of bi-directional thermal management in improving component reliability. By offering a robust combination of high-resolution characterization, advanced simulation, and intelligent data modelling, the study sets a foundation for data-augmented digital twin frameworks aimed at the next generation of AM process design for critical high-temperature applications.

1.5 Research Objectives

The fabrication of 9Cr-1Mo steel components using CMT-based DED presents a promising route for developing high-temperature structural parts with complex geometries. However, the process is accompanied by critical challenges, including non-uniform thermal cycles, uncontrolled phase transformations, and high residual stress accumulation, all of which adversely affect the microstructural stability and mechanical performance of the final build, particularly under creep conditions. These issues stem from the complex interplay between heat input, scan strategy, inter-layer interactions, and transformation-induced strains. To address these challenges, the present study is structured around the following three objectives, which integrate experimental characterization, computational modeling, and artificial intelligence (AI) to provide a holistic understanding and control framework for the deposition process.

- **Characterization of 9Cr-1Mo steel deposits made by DED of CMT process**

To experimentally evaluate the deposition characteristics of 9Cr-1Mo steel using CMT-based DED by fabricating single bead, multi-track, and multi-layer structures under various scan strategies. Detailed characterization includes optical microscopy, SEM, EBSD, XRD, and dilatometry, along with EDS for identifying $M_{23}C_6$ and MX precipitates. Microhardness testing is conducted to assess property gradients, while portable XRD is used to measure residual stress in the printed components. Fractography of tensile-tested specimens is performed to analyze failure modes and crack initiation due to residual stress. This comprehensive evaluation links processing conditions with microstructural evolution, mechanical behavior,

and residual stress development.

- **Finite element-based modeling of thermo-metallurgical-mechanical behavior**

To develop a finite element-based TMM model capable of simulating transient thermal fields, phase transformations, and residual stress evolution in the CMT-based DED process. The model incorporates temperature-dependent material properties, martensitic transformation kinetics, and transformation-induced plasticity. It serves as a predictive tool to study the effects of inter-layer dwell time, scan path strategy, and process parameters on the evolution of thermal and mechanical fields.

- **AI-driven forward and backward prediction of temperature and residual stress field**

To complement computationally expensive FE simulations with physics-informed machine learning and deep learning approaches for rapid and accurate prediction of process responses. AI models are first employed to predict transient thermal and residual stress profiles; DL frameworks are then applied to capture the role of inter-layer dwell time on thermo-mechanical responses; and TCN models are finally used to predict dilatometric responses. Together, these models establish a computationally efficient and predictive framework that accelerates the development of a thermo-metallurgical-mechanical model and guides the optimization of deposition strategies for improved performance.

1.6 Layout of Thesis

The thesis comprises six interconnected chapters, each contributing to a comprehensive investigation into the deposition behaviour of 9Cr-1Mo steel using CMT-based DED. **Chapter 1** introduces the background of the research problem, highlighting the critical challenges associated with residual stress, phase transformation, and microstructural non-uniformity in arc-based AM process. It presents the motivation, research objectives, and the overall structure of the thesis. Building upon this foundation, **Chapter 2** offers an extensive review of the current state of research, focusing on experimental studies, numerical modelling of thermal and residual stress evolution, and the application of AI models for predictive analytics in metal AM. Special attention is given to the capabilities of CMT-based DED in mitigating Type IV cracking in 9Cr-1Mo steel components. **Chapter 3** then outlines the experimental methodology, including the selection of deposition parameters, fabrication of various build geometries (single bead, multi-track, multi-layer), and implementation of advanced scan

strategies such as uni-/bi-directional, spiral, inclined, and circular paths. This chapter also details the use of high-resolution characterization techniques including SEM, EBSD, XRD, EDS, dilatometry, microhardness testing, and tensile testing, along with fractographic analysis to understand failure mechanisms and stress-induced crack initiation. **Chapter 4** transitions into the computational aspect by developing a finite element-based TMM model capable of simulating transient temperature fields, martensitic transformation, and residual stress, incorporating temperature-dependent properties and transformation-induced plasticity. In parallel, the chapter describes the construction of physics-informed deep learning (PIDL) models, elaborating on dataset formulation, preprocessing, model training, and performance evaluation, including a comparative assessment of different architectures. **Chapter 5** consolidates the findings through a detailed discussion of model validation and result interpretation. The TMM model is validated using experimental data for different deposition configurations, and the effects of heat input, inter-layer dwell time, and scan patterns on thermal and mechanical behaviour are critically analysed. Simultaneously, the PIDL models are used to predict nonlinear thermal and residual stress profiles, with optimized predictions guiding the selection of inter-layer dwell times to limit residual stress below the yield strength of 9Cr-1Mo steel. Furthermore, temporal convolutional networks (TCNs) are trained on dilatometric strain datasets to capture the influence of scan paths on transformation strain, and these models are then employed to design optimized scanning strategies using simulated thermal data. Finally, **Chapter 6** summarizes the major outcomes of the research, reflects on the scientific contributions, and outlines future research directions, followed by a detailed list of references that support the entirety of the study.



Chapter 2

Literature Survey

2.1 General background

Fabrication of product by wire-based DED process can be broadly categorized into three interconnected phases: the design phase, the processing phase, and the testing phase. Each phase plays a critical role in determining the quality, structural soundness, and performance reliability of the final component. A clear understanding and precise execution of these stages are essential, particularly when fabricating components from high-performance alloys like 9Cr-1Mo steel, which are sensitive to thermal and mechanical processing conditions. The design phase (Phase-1) forms the foundation of the entire DED workflow. It begins with defining the specifications and requirements of the component based on its intended function, environmental exposure, and mechanical performance. Once the design intent is clear, the component geometry is developed using computer-aided design (CAD) software. The CAD model is then converted into a standard tessellation language (STL) file, which represents the 3D geometry as a mesh of triangles suitable for additive manufacturing. This file is subsequently transferred to the deposition system, where it undergoes slicing into a series of discrete layers and toolpath generation tailored to the selected DED strategy. The output of this phase determines the resolution, layer thickness, build direction, and overall fidelity of the component.

Following the digital preparation, the processing phase (Phase-2) involves the physical building of the component layer by layer (Figure 2.1). This begins with the setup of deposition parameters on the machine, such as wire feed rate, travel speed, arc voltage, current, inter-layer

dwelt time, and shielding gas composition. These parameters collectively define the thermal field, melt pool dynamics, and deposition characteristics such as bead shape, dilution, and surface finish. Once the parameters are configured, the DED machine initiates the deposition process, where metallic wire is melted by an electric arc and deposited along the predefined toolpaths to build the component in a layer-wise manner. Upon completion, the component is removed from the substrate and typically undergoes post-processing operations including heat treatment, surface machining, or stress-relieving, depending on the application-specific requirements. The final step, the testing phase (Phase-3), focuses on the evaluation of the fabricated component. The as-built part undergoes geometric inspection and non-destructive testing to verify whether it conforms to the dimensional tolerances, mechanical properties, and microstructural standards specified during Phase-1. If the component meets the specification limits, it is accepted and proceeds to service or further processing. However, if it falls outside the defined quality window, the part is rejected, and the process feedback is analysed. In such cases, process parameters are recalibrated.

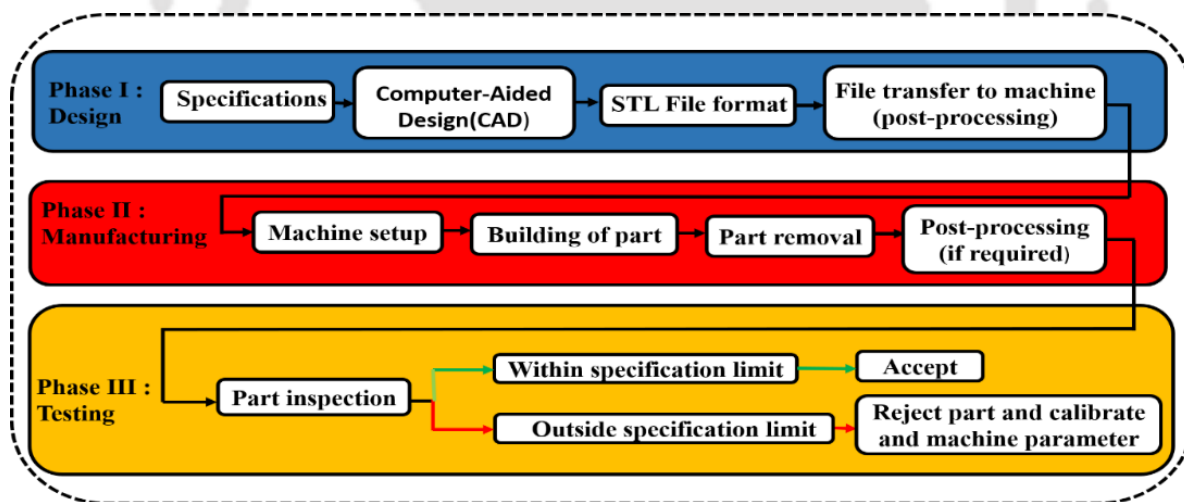


Figure 2.1: Schematic representation of the additive manufacturing workflow comprising the design phase, manufacturing phase, and testing phase [75].

Within the evolving landscape of metal-based AM process, DED, particularly arc-based variants such as CMT have garnered increasing attention for its unique capabilities in fabricating large scale, functional metallic components. While PBF remains prominent for producing fine featured and high-resolution parts, especially in the biomedical and aerospace

sectors, it presents inherent limitations in terms of build volume, powder reuse, and equipment cost. In contrast, arc-based DED offers a robust and economically viable solution for structural applications where dimensional scale, mechanical integrity, and deposition rate take precedence over fine resolution. Arc based DED employs a high efficiency electric arc as the energy source and utilizes wire feedstock instead of powder, enabling better material utilization, reduced operational hazards, and significantly lower raw material costs. This wire-based approach also eliminates powder related challenges such as oxidation, flowability, and safety concerns, thereby expanding the range of weldable and reactive alloys that can be processed. Moreover, the high deposition rates achievable with arc-based DED, often an order of magnitude greater than those of PBF, make it particularly attractive for producing near net shape components with reduced manufacturing time. Another distinct advantage of arc-based DED lies in its scalability and flexibility. The open architecture nature of DED systems allows for integration with robotic arms or gantry systems, enabling deposition on non-planar surfaces or the repair of damaged parts, capabilities that are difficult to achieve using PBF. Furthermore, the layer wise thermal input in arc DED can be precisely tailored by controlling travel speed, arc current, and interlayer dwell time, allowing fine control over microstructural evolution, residual stress development, and phase transformation behaviour, particularly critical for thermally sensitive alloys such as 9Cr 1Mo steel.

Table 2.1 provides a comparative summary of arc-based DED and PBF, illustrating key differences in energy source, feedstock form, deposition rate, build volume, and application domain. While PBF excels in micro feature resolution and is suitable for small, intricate components with tight tolerances, arc-based DED is clearly superior when it comes to producing large, structurally robust parts at low cost and high throughput, particularly in sectors such as power generation, oil and gas, and heavy engineering. In summary, the advantages of low feedstock cost, high material deposition rates, reduced system complexity, and suitability for large scale builds make arc-based DED a compelling technology for the fabrication and repair of high-performance ferritic steels. These strengths align directly with the objectives of the present study, which focuses on tailoring and optimizing the deposition characteristics of 9Cr 1Mo steel components using an arc-based DED process.

Table 2.1: A Comparison of two main categories of AM for metallic components: DED and PBF [1].

AM process	DED			PBF	
Feed stock material	Powder	Wire		Powder	
Heat source	Laser	E-beam	Electric arc	Laser	E-beam
Nomenclature	DED-L	DED-EB	DED- - GMA	PBF-L	PBF-EB
Power(W)	100-3000	500-2000	1000–3000	50–1000	50–1000
Maximum feed rate	0.1-1.0	0.1-2.0	0.2–2.8	-	-
Maximum build size ($mm \times mm \times mm$)	2000×1500×750	2000×1500×750	5000×3000×1000	50×280×320	50×280×320
Speed (mm/s)	5-20	1-10	5-15	10-1000	10-1000
Production time	High	Medium	Low	High	High
Surface roughness (μm)	4-10	8-15	Needs machining	7-20	7-20
Dimensional accuracy(mm)	0.5-1.0	1.0-1.5	Intricate features are not possible	0.04-0.2	0.04-0.2
Post processing	H.I.P. and surface grinding	Surface grinding and machining	Machining is essential	H.I.P.	H.I.P

2.2 Evolution of ferritic steel

Creep Strength Enhanced Ferritic (CSEF) steels have emerged as the most promising class of materials for structural components in advanced ultra-supercritical (AUSC) power plants, where prolonged exposure to elevated temperatures and pressures demands superior creep resistance, oxidation stability, and dimensional reliability. Their adoption in steam piping, headers, and pressure vessels has been driven by the need to sustain operating temperatures up to 620 °C and pressures exceeding 27.6 MPa, while maintaining mechanical integrity and minimizing component deformation over long service durations. These steels offer several advantages over conventional materials, including higher thermal conductivity, lower thermal expansion, and significantly reduced material costs when compared to austenitic stainless steels. The development of CSEF steels is rooted in the gradual evolution of ferritic Cr–Mo steel compositions, which began with traditional 2.25Cr–1Mo steels and progressed toward advanced 9–12Cr alloys tailored for elevated temperature service. The alloying strategy has primarily focused on enhancing long-term creep strength while maintaining weldability and oxidation resistance. As illustrated in Figure 2.2, this progression has involved strategic modifications in base composition and the incorporation of strengthening elements such as vanadium (V), niobium (Nb), boron (B), and nitrogen (N). These refinements have enabled the development of several advanced grades including T/P23, T24, E911, P(T)91, P(T)92, P(T)122, and VM12SHC each addressing specific performance criteria required for next-generation thermal systems. Among these, 9Cr-1Mo steel (P91) stands out due to its widespread use and excellent balance of mechanical properties and thermal stability. Originally developed in the 1970s at Oak Ridge National Laboratory for nuclear applications, P91 was later standardized by ASTM and ASME in 1984 and became a key material for fossil-fired power plant piping, tubing, and headers. Its tempered martensitic microstructure, coupled with a well-dispersed population of strengthening precipitates such as $M_{23}C_6$ carbides and MX-type carbonitrides, provides high creep resistance and oxidation stability during long-term service. The subsequent evolution of P92 steel, incorporating tungsten (W) in place of molybdenum (Mo) along with controlled additions of B and N, further enhanced high-temperature performance and extended application limits.

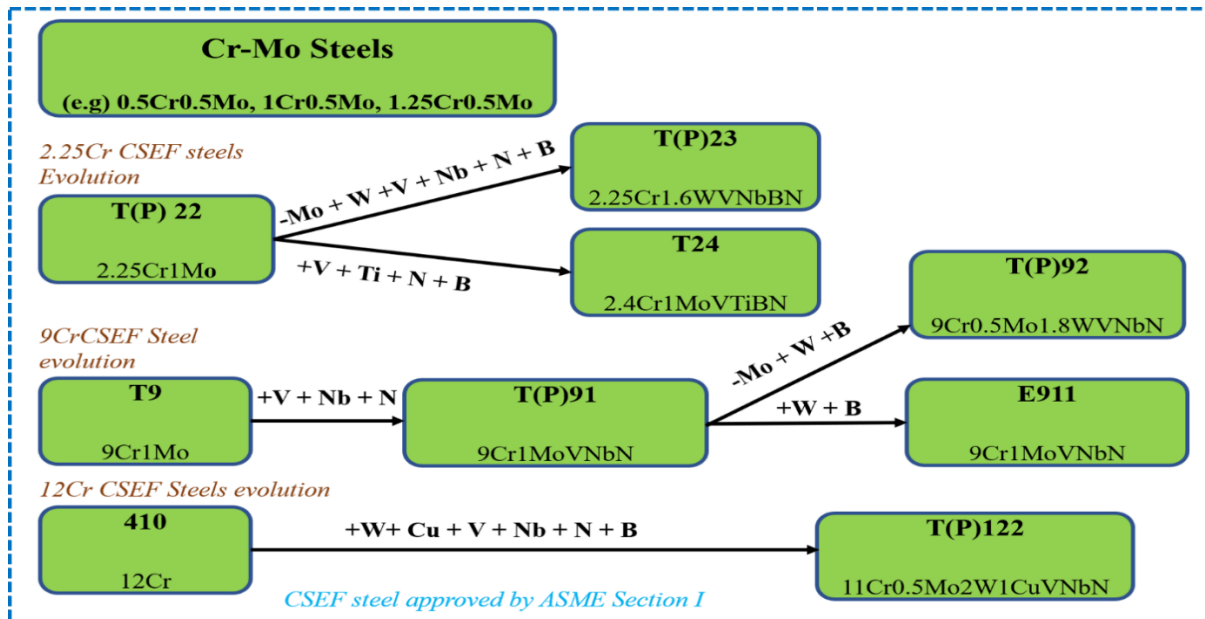


Figure 2.2: Evolution of different grades of ferritic steel on the modification of key elements for high temperature applications [3].

Despite the superior high-temperature capabilities of CSEF steels like P91 and P92 are not immune to degradation mechanisms, particularly in the heat-affected zones (HAZ) of welded joints. One of the most critical challenges observed during long-term operation is Type IV creep failure, which occurs due to localized softening in the fine-grained HAZ region. This phenomenon is primarily attributed to the inability of the material to recover its original tempered martensitic microstructure after welding or post-weld heat treatment. The degradation is further accelerated by the coarsening of $M_{23}C_6$ precipitates, dissolution or instability of MX particles, and the formation of creep cavities along grain boundaries. To address these concerns, ongoing alloy development has introduced 12Cr variants, such as VM12SHC, designed to improve oxidation resistance while maintaining creep strength. However, limitations such as restricted wall thickness and weldability persist. The effective deployment of 9Cr-based CSEF steels thus requires a comprehensive understanding of their microstructural evolution, precipitate stability, and damage mechanisms particularly when exposed to cyclic thermal loads or processed via additive manufacturing routes like arc-based DED, where repeated thermal cycles can exacerbate Type IV cracking susceptibility.

2.3 Deposition characteristics

Deposition characteristics in arc-based DED process play a pivotal role in determining the quality, performance, and dimensional accuracy of the fabricated component. These characteristics result from the complex interplay between process control parameters, the underlying thermal and mechanical phenomena during deposition, and the resulting geometrical features of the build (Figure 2.3). At the foundation are the deposition attributes, which include critical build setup parameters such as shielding gas flow, inter-layer dwell time, and inter-layer temperature. These variables directly affect the thermal stability of the process; for instance, inadequate gas shielding can lead to oxidation, while improper dwell time may cause excessive heat accumulation, adversely influencing inter-layer bonding and microstructural uniformity. Simultaneously, the heat input regulated by arc voltage, current, and travel speed dictates the melt pool size and energy distribution. Excessive heat input can lead to melt pool instability, increased dilution, and unwanted remelting of underlying layers, whereas insufficient energy input often causes incomplete fusion, leading to porosity and lack of bonding. The nature of the consumables, including wire diameter, wire feed speed, and shielding gas composition, further impacts arc stability and deposition behavior. For example, using a larger diameter wire demands higher current and feed rates to maintain a stable arc and consistent material transfer, while the choice of gas mixture affects arc temperature, cooling rate, and oxidation tendency. Path planning, which includes slicing strategy and toolpath generation, also significantly influences heat distribution, melt pool evolution, and solidification dynamics. Poor paths overlap or inefficient slicing can cause irregular thermal gradients, which may induce directional solidification, non-uniform grain growth, or residual stress accumulation. To mitigate such effects and enhance microstructural control, post-deposition treatments such as inter-pass heating or cooling and cold working are often applied. These measures help manage the thermal field across layers, stabilize microstructure, and improve mechanical performance.

Physical phenomena that unfold during depositions such as reheating and remelting cycles, steep thermal gradients, fluctuating cooling rates, and melt pool behavior directly affect phase transformation kinetics and residual stress evolution. In ferritic steels like 9Cr-1Mo, these repeated thermal cycles can destabilize the martensitic matrix, affect precipitate morphology (including $M_{23}C_6$ carbides and MX-type carbonitrides), and alter the overall microstructural

integrity of the build. The repeated application and extraction of heat across layers result in differential expansion and contraction, which give rise to stress accumulation and strain localization. If unchecked, these residual stresses can cause part distortion, inter-layer delamination, or even cracking particularly within the heat-affected zone where softened grains become susceptible to Type IV creep failure. Influence of these phenomena becomes evident in the final geometrical features of the component. Key outputs such as track width and height, build height uniformity, and surface finish are all determined by the synergy between heat input, material flow, and thermal behavior. Non-uniform tracks can lead to cumulative dimensional errors, underfilled or overbuilt sections, and loss of part accuracy. In addition, rough surfaces, often caused by arc spatter or inconsistent solidification fronts, degrade fatigue life and necessitate extensive post-processing. Challenges intensify when printing overhangs or unsupported geometries, as improper heat dissipation and melt pool instability in these regions demand precise tuning of path strategies and energy input. Another critical defect is porosity that is tightly linked to the combined effects of fusion quality, gas shielding effectiveness, and melt pool control. Porosity compromises mechanical performance and is often rooted in energy imbalance, shielding gas turbulence, or improper re-melting. Ultimately, all these aspects of deposition are inherently interdependent. A deviation in any parameter such as heat input, dwell time, wire feed rate, or path strategy can cascade through the process, altering the thermal profile, residual stress field, and final part geometry. Therefore, achieving high-quality and structurally robust builds in arc-based DED necessitates a holistic and integrated understanding of how deposition characteristics influence thermal cycles, microstructural evolution, and geometrical fidelity.

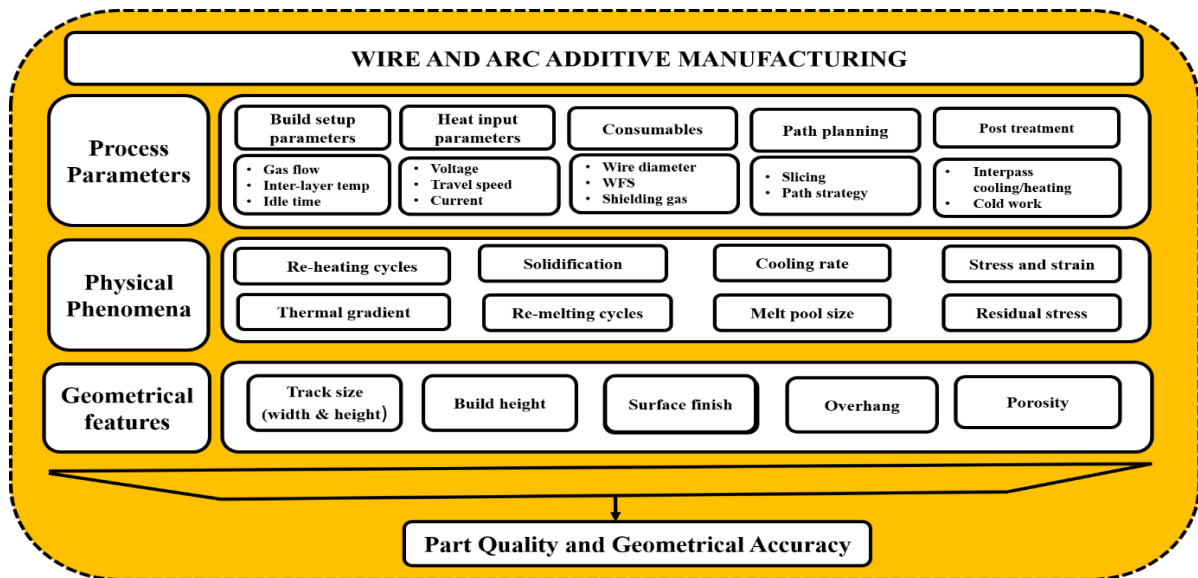


Figure 2.3: Essential required for controlling the fabrication quality in arc-based AM process.

2.4 Residual stress evolution in wire-based DED process

In arc-based DED, the evolution of residual stress is inherently governed by the complex interplay of localized heat input, rapid thermal cycling, constrained thermal expansion, and microstructural transformations. The process involves successive deposition of molten material onto a substrate using an electric arc as the heat source. This localized and repeated heating leads to steep thermal gradients between the deposited layers and the surrounding substrate, resulting in heterogeneous thermal expansion and contraction. During deposition, the arc-induced heat rapidly elevates the temperature of the feedstock and substrate beyond their melting and solidification points, respectively, forming a molten pool that solidifies upon the arc's traversal. However, this thermal input is far from uniform, and the regions adjacent to the melt pool particularly the previously deposited layers and the underlying substrate remain relatively cooler, thereby resisting the expansion of the hot zone. This restraint causes the accumulation of thermal stresses in the vicinity of the melt pool. As the heat source progresses, the previously molten region undergoes rapid cooling, triggering solidification followed by contraction. Due to the mechanical constraint provided by the surrounding cooler material, this contraction does not proceed freely, and tensile residual stresses develop in the deposited layers. Simultaneously, compressive stresses form in the surrounding regions to

maintain internal equilibrium. This effect is cumulative with each subsequent layer, leading to a complex three-dimensional stress field throughout the build.

Additionally, the thermal cycle in DED often causes solid-state phase transformations such as martensitic transformation in steels which are accompanied by volumetric changes. When such transformations induce expansion in a constrained environment, compressive residual stresses may form in the transformed zone, while balancing tensile stresses may appear in the adjacent areas. Thus, the residual stress pattern is not only influenced by thermal contraction but also by the kinetics and magnitude of phase transformation-induced volume change. Moreover, the temperature-dependent nature of material properties such as yield strength plays a critical role. At elevated temperatures, materials exhibit reduced yield strength, making them susceptible to plastic deformation under relatively low thermal stresses. Upon cooling, these plastically deformed zones experience elastic mismatch with adjacent elastic regions, giving rise to permanent residual stress. As layer-by-layer deposition progresses, the thermal history of previously deposited material evolves, causing partial stress relaxation in some regions and stress accumulation in others, depending on their thermal exposure and degree of constraint. Another contributing factor is the scan strategy and path planning, which determine how heat is distributed over the deposition area. Continuous unidirectional scanning may result in asymmetric heat accumulation and produce higher residual stresses along the scanning direction. In contrast, alternate or bidirectional scanning can balance the thermal field, potentially reducing residual stress buildup. Additionally, geometrical features such as overhangs, thin walls, and varying cross-sections introduce uneven thermal conductivity paths, further exacerbating residual stress heterogeneity.

From a mechanistic viewpoint, the evolution of residual stress in arc-based DED follows a sequence beginning with thermal agitation in the localized arc-affected zone, followed by melt pool formation, solidification, and subsequent solid-state transformation. These thermal and phase-related processes introduce macrostrain due to incompatible lattice distortions, especially in regions undergoing differential cooling or dissimilar transformation kinetics. Over time, this macrostrain accumulates, influencing both the magnitude and distribution of residual stresses. On a microstructural scale, residual stresses are also influenced by heterogeneous grain structures and dislocation densities, especially in multi-pass deposition where thermal cycles affect grain refinement and phase stability. Based on the spatial scale of

stress distribution, residual stresses in DED-fabricated components can be broadly classified into Type I (macro-stress), Type II (intergranular microstress), and Type III (intragranular microstress). Type I stresses span across multiple deposition layers and are largely influenced by thermal gradients and constraint conditions. Type II stresses arise from differences in elastic or thermal properties between grains of varying orientations, typically due to texture development during rapid solidification. Type III stresses, on the other hand, stem from lattice-scale imperfections such as dislocations, precipitates, or inclusions introduced during solidification and thermal cycling. In summary, the evolution of residual stress in arc-based DED is a result of multi-scale, thermomechanical interactions involving localized heating, constrained thermal expansion and contraction, temperature-dependent plasticity, and phase transformation-induced volumetric changes. The resulting stress field is spatially heterogeneous and evolves both within and across layers, significantly impacting the structural integrity, dimensional stability, and service performance of the fabricated component. Therefore, understanding and controlling residual stress through process optimization, scan strategy design, and thermal management is essential for achieving high-quality and defect-free AM structures.

2.4.1 *Measurement of residual stress*

In the context of AM process, particularly arc-based DED, the measurement of residual stress is vital for assessing part quality, dimensional accuracy, and long-term performance. The thermal cycling inherent to layer-by-layer deposition induces complex stress fields that vary both spatially and temporally. Experimental quantification of these stresses enables validation of predictive models and guides optimization of process parameters. Broadly, residual stress measurement techniques can be categorized into destructive, semi-destructive, and non-destructive approaches, each offering unique advantages depending on resolution, depth sensitivity, and applicability to AM components. Among the semi-destructive techniques, hole-drilling stands out as one of the most widely adopted methods due to its operational simplicity and ability to provide near-surface residual stress profiles. In this method, a small hole is incrementally drilled at the center of a strain gauge rosette affixed to the surface of the deposited sample. The relaxation of pre-existing stresses due to material removal leads to strain redistribution, which is captured by the strain gauges. These measurements are then used to

back-calculate the original residual stress components. This technique is particularly suitable for assessing layer-wise stress evolution in arc-based DED builds, where thermal gradients and layer interactions play a significant role in stress development. Ring-core and deep-hole drilling methods are further advancements of the hole-drilling technique. The ring-core method involves machining an annular groove around a central core to evaluate deformation-induced stress relief, allowing deeper penetration compared to conventional hole drilling. The deep-hole drilling method, on the other hand, enables through-thickness stress profiling by measuring dimensional changes of a pre-drilled hole before and after trepanning the surrounding core. This method is highly effective for large-scale arc-based DED structures where stress evolution along the build height is of interest. Fully destructive techniques such as the contour method have proven especially valuable for assessing two-dimensional distribution of stress distributions in AM components. This method involves precisely sectioning the sample through the region of interest using wire electrical discharge machining (EDM), followed by surface profiling of the newly exposed face using coordinate measurement or laser scanning tools. The surface deformation profile, caused by stress relaxation during cutting, is used to reconstruct the original residual stress field via finite element-based inverse analysis. This technique has been successfully applied in the characterization of WAAM-fabricated aluminum and steel components, providing deep insight into the internal stress states without the need for pre-applied sensors or gauges.

The X-ray diffraction (XRD) technique is a widely adopted non-destructive method for evaluating surface-level residual stress in crystalline materials, particularly in metallic components fabricated through AM processes such as wire-based DED. This technique operates on the fundamental principle that residual stresses alter the atomic lattice spacing within a crystalline structure, leading to measurable shifts in the diffraction angle. Metals, being composed of atoms arranged in a regular periodic lattice, exhibit well-defined interplanar spacings that diffract X-rays according to Bragg's Law. When residual stresses are present, these spacings deviate from their stress-free values, thereby modifying the conditions under which diffraction occurs. Bragg's Law, defined by

$$2d_{hkl}\sin\theta = n\lambda \quad (2.1)$$

where d_{hkl} denotes the interplanar spacing of the crystal planes, θ is the Bragg angle, λ is the wavelength of the incident X-rays, and n is the order of diffraction. When a material is subjected to internal stress, the interplanar spacing d_{hkl} either expands or contracts, which in turn causes a corresponding change in the measured diffraction angle θ . The elastic strain ε induced by residual stress is then computed as the relative change in interplanar spacing, expressed as

$$\varepsilon = \frac{(d_{hkl} - d_0)}{d_0} \quad (2.2)$$

where d_0 is the stress-free spacing.

To fully characterize the stress tensor, measurements must be performed at various orientations of the sample with respect to the incident X-ray beam. This is commonly achieved using the $\sin^2\psi$, where ψ is the angle between the sample surface normal and the diffraction vector and ϕ represents the azimuthal angle within the sample surface. The measured strain in the diffraction direction for a given orientation (ϕ, ψ) is a combination of the in-plane and out-of-plane strain components. For the evaluation of strain tensors at any sampling gauge location, measurement of strain in different directions are estimated as

$$\varepsilon(\phi, \psi) = \varepsilon_{11}\cos^2\phi\sin^2\psi + \varepsilon_{22}\sin^2\phi\sin^2\psi + \varepsilon_{33}\cos^2\psi + \varepsilon_{12}\sin 2\phi\sin^2\psi + \varepsilon_{13}\cos\phi\sin 2\psi + \varepsilon_{23}\sin\phi\sin 2\psi \quad (2.3)$$

Once the strain tensor is known, the corresponding stress components are computed using the generalized Hooke's law adapted for crystallographic directions. Assuming linear elasticity and isotropy in the measurement direction, the stress-strain relationship is given by

$$\sigma_{ij} = \left(\frac{E_{hkl}}{1 + \nu_{hkl}} \right) \left(\varepsilon_{ij} + \frac{\nu_{hkl}}{1 - 2\nu_{hkl}} \varepsilon_{kk} \delta_{ij} \right) \quad (2.4)$$

where E_{hkl} and ν_{hkl} are the elastic modulus and Poisson's ratio for the (hkl) planes, respectively. Here, ε_{kk} denotes the trace of the strain tensor (i.e., the sum of the normal strains), and, δ_{ij} is the Kronecker delta, which simplifies the relation in Cartesian form. In practical

applications involving additively manufactured components, especially those produced by arc-based DED, the principal stress directions often align with the build and scanning axes. In such cases, symmetry assumptions can reduce the complexity of the measurements, allowing residual stresses to be determined using a limited number of strain measurements. For instance, under the assumption of principal stress alignment and elastic isotropy, the principal residual stress can be evaluated from the relation

$$\sigma_{11} = \frac{E_{hkl}}{(1 - \nu_{hkl})(1 - 2\nu_{hkl})} [(1 - \nu_{hkl})\varepsilon_{11} + \nu_{hkl} (\varepsilon_{22} + \varepsilon_{33})] \quad (2.5)$$

2.4.2 *Martensitic transformation induced residual stress*

9Cr–1Mo steel, a ferritic-martensitic composition, is extensively utilized in AUSC power plants owing to its exceptional creep resistance, oxidation tolerance, and thermal stability at elevated temperature. The microstructure composed of tempered martensite with finely dispersed $M_{23}C_6$ carbides and MX-type precipitates, ensures long-term mechanical integrity under harsh service conditions [76,77]. However, during arc-based DED, the material is subjected to rapid heating and cooling cycles, leading to solid-state austenite-to-martensite transformation accompanied by a volumetric expansion [1,10]. While this transformation contributes to strength enhancement, it also induces substantial tensile residual stresses by constrained thermal contraction during cooling. This tensile residual stress may compromise the structural reliability of components, particularly in the heat-affected zone, where it facilitates localized creep damage and premature failure commonly referred to as Type IV cracking [3,78]. Such cracking is especially critical in manufacturing components of layer-by-layer deposition process, where mechanical integrity is vital over prolonged high-temperature exposure. As a result, understanding the thermal and phase transformation history during deposition is essential to minimize stress accumulation and ensure dimensional accuracy and mechanical performance of 9Cr–1Mo steel builds.

The generation of tensile residual stress is fundamentally governed by steep thermal gradient and non-uniform cooling that occur during the rapid solidification of deposited material. These stresses arise due to constrained thermal contraction between successive layers and tracks, especially in multi-track, multi-layer builds where heat accumulation and cyclic reheating become prominent [35,79]. It is apparent that the scanning strategy plays a pivotal

role in regulating the spatiotemporal distribution of heat, which directly influences the evolution of residual stress [80,81]. Prior investigations have demonstrated that the adoption of non-linear scan paths such as bidirectional raster, checkerboard, inclined, or rotated strategies can significantly alleviate directional heat buildup and promote uniform thermal fields [82,83]. A study reported by sun et al. [84], zigzag and spiral strategies yield lower residual stress magnitudes compared to unidirectional raster due to their ability to redistribute heat and promote isotropic shrinkage. Such strategies facilitate stress relaxation mechanisms and disrupt the formation of high-stress concentration zones, ultimately enhancing the dimensional accuracy and structural integrity of arc-DED-fabricated components. Moyle et al. [85] printed martensitic stainless steel under different laser powers and scanning strategies (hexagonal, raster, concentric). It is concluded that higher heat input improves ductility along the build direction. However, the solution annealing induces austenite phase that enhances work hardening via the TRIP effect. Critically, scanning strategy has a stronger influence on residual stress than heat input. The concentric scans produce the highest stress, making raster and hexagonal strategies more favorable for minimizing stress buildup. Nadammal et al. [86] shows that the scan strategies such as alternating and rotational patterns effectively controls the residual stress and texture in deposited Inconel 718. The rotational strategy generates the most random grain orientations and lowest residual stress, while short hatch length strategies induces higher anisotropy and stress gradients. These findings emphasize that careful pre-processing design of scan paths and hatch settings can minimize distortion and reduce reliance on costly post-processing techniques. The Ti-6Al-4V parts fabricated on varying scanning strategies depicts that a 45° scan with 90° -layer rotation significantly reduces through-thickness residual stress by promoting a more uniform thermal profile [87]. These findings offer significant routes for optimizing scan strategies to minimize stress gradients, especially in thicker components.

The martensitic transformation during in-process reheating plays a central role in enhancing the fatigue life of as-printed martensitic M789 steel by generating beneficial compressive residual stress surface [88]. When reheating occurs below the martensitic start temperature, the associated constrained volume expansion from austenite-to-martensitic transformation induces compressive stresses resulting in up to a 600% increase in fatigue life compared to as-built samples. This beneficial role of martensitic transformation is not limited

to steels. In high- and medium-entropy alloys (MEAs) such as $\text{Co}_{45}\text{Cr}_{25}(\text{FeNi})_{30}$, martensitic transformation also plays a critical role in enhancing mechanical performance [89]. In this alloy, stress-assisted martensitic transformation activated well below the macroscopic yield stress driven by residual stress and dislocation density from rapid solidification triggers the TRIP effect, enabling progressive strain hardening and mitigating plastic anisotropy. Thus, whether triggered thermally in steel to induce compressive residual stress or mechanically in MEAs to enhance ductility and isotropy, martensitic transformation, combined with residual stress control, offers a versatile approach for optimizing the performance of AM alloys.

2.4.3 Mitigation of residual stress

Residual stress mitigation in arc-based DED is critical to ensuring the dimensional stability, mechanical integrity, and long-term performance of additively manufactured components, particularly those involving thin walls, large surfaces, or intricate geometries commonly used in aerospace, shipbuilding, and high-performance structural applications. During DED, residual stresses primarily originate from the highly localized and cyclic heat input associated with the arc source, which creates steep thermal gradients and non-uniform cooling rates. These thermal cycles induce incompatible plastic strains between the molten zone, the heat-affected zone, and the base metal, leading to tensile and compressive stress distributions that persist after solidification and cooling. Therefore, to minimize the development and accumulation of these stresses, a combination of intelligent deposition strategy modulation, precise control of process parameters, and targeted post-deposition treatments must be implemented. A fundamental approach to mitigating residual stress lies in the optimization of the deposition strategy, which governs the spatial and temporal evolution of heat within the build. Traditional unidirectional raster patterns tend to accumulate heat in localized regions, leading to asymmetric stress development and distortion. To overcome this, advanced strategies such as bidirectional scanning, interleaved deposition, island-based partitioning, and segmental reciprocating motion are employed. These strategies aim to redistribute the thermal load across the build area, thereby avoiding excessive heat buildup and allowing for more uniform cooling. For instance, segmental reciprocating motion divides the layer into smaller segments, depositing each in alternating directions to ensure a more balanced temperature field. This not only suppresses the formation of residual tensile stress peaks near

the weld line but also reduces the thermal accumulation between layers, which is often a major contributor to distortion.

In parallel, fine-tuning of process parameters plays a critical role in influencing melt pool behaviour, cooling rates, and the resulting thermal stress fields. Parameters such as arc power, travel speed, wire feed rate, and inter-layer dwell time directly affect the heat input and thermal cycles experienced by the material. By reducing the arc power or increasing the travel speed, the input energy density can be minimized, resulting in a smaller and more stable melt pool. A reduced melt pool size decreases the extent of the heat-affected zone and lowers the thermal gradient between the deposited layer and the surrounding material, thus mitigating residual stress development. Equally important is the inter-layer dwell time, which governs the time allowed for a previously deposited layer to cool before the next is deposited. Sufficient dwell time facilitates more uniform temperature distribution through the thickness, promoting gradual thermal contraction and thereby reducing stress accumulation across the build height. Conversely, inadequate dwell time can lead to thermal accumulation, steep gradients, and stress intensification, especially near the fusion boundaries. Despite all efforts to control residual stress during deposition, some amount of stress is inevitably retained within the structure. For this reason, post-deposition mitigation techniques are often employed as a complementary approach. One widely used method is mechanical rolling, which can be applied layer-wise or after full part fabrication. The plastic deformation introduced by rolling compresses the surface layers, resulting in the redistribution of internal stresses and often reversing the tensile stress state into a more favourable compressive one. This technique also refines the grain structure, enhances surface hardness, and improves fatigue resistance. Another effective technique is post-deposition heat treatment, including stress-relief annealing and solution treatment, which enables atomic diffusion and dislocation recovery, leading to a homogenization of internal strains and a significant reduction in residual stresses. The thermal cycle during heat treatment must be carefully designed to avoid overaging or grain coarsening, especially in alloys prone to phase instability. Moreover, more advanced post-deposition techniques such as laser shock peening (LSP), ultrasonic impact treatment (UIT), and hammer peening have been increasingly integrated into the DED workflow. These techniques apply localized mechanical or laser-induced shockwaves to the component surface, introducing compressive residual stresses in the near-surface region and thereby counteracting the inherent

tensile stresses induced during the build. For example, LSP delivers high-pressure plasma-generated shockwaves that plastically deform the surface layer without significant thermal input, making it ideal for fatigue-sensitive aerospace components. Similarly, vibration-assisted processing during or after deposition has shown promise in relaxing stress through cyclic plastic strain, enhancing the overall stress state of the build.

Collectively, the mitigation of residual stress in arc-based DED is not reliant on a single intervention, but rather on a multi-faceted strategy that begins with intelligent planning of deposition sequences, continues through meticulous control of process variables, and is completed with effective post-processing. This integrated approach enables the production of structurally sound, geometrically accurate, and performance-optimized components, fulfilling the stringent requirements of high-reliability industries. Furthermore, the continuous development of real-time monitoring and adaptive control techniques such as thermographic imaging, closed-loop heat input control, and in-situ stress sensing holds the potential to further advance stress mitigation by providing feedback during the deposition process itself, ultimately enabling a transition from reactive to proactive stress management in AM process.

2.5 Numerical modelling of WAAM process

Numerical modeling of the arc-based AM process plays a key role in product development, i.e., from designing of product to process planning, monitoring, and control; these techniques help to mitigate common WAAM defects and increase the qualification of the produced part [90]. For developing a computational model of the direct energy deposition (DED.) process, which consists of modeling of moving heat and mass source in the form of wire, such simulation considers the thermal history, melting and solidification cycles, and effect of various deposition strategies [91]. A selection of various numerical models for simulating different physical phenomena and different geometrical features for wire-based DED processes are shown in Table 2.2.

Table 2.2: Various numerical modeling techniques are utilized for simulating the arc WAAM process.

Objective	Modelling technique	Characteristics	Application of numerical model
Calculation of heat, mass, and momentum transfer	Using Fourier heat conduction model	Fourier heat conduction models are solved either analytically or numerically by using commercial software This modeling technique does not consider the molten metal flow inside the weld pool and frequently gives the inadequate thermal profile	Temperature distribution [92],[34] Solidification parameters [93,94]
	Heat transfer and fluid flow model	Solution of 3D conservation equations of mass, momentum, and energy equation is required. It considers the flow of molten metal inside the pool.	Temperature and velocity field [95,96]
	The volume of the fluid and level set methods	To track the dynamics of the free surface of the molten metal	Deposition geometry [32,96]
Computation of residual stress and distortion	Thermomechanical model using finite element analysis	3D constitutive equations which consider elastic, plastic, and thermal are solved	Residual stresses [49,50,51] Distortion [97],

			delamination [98], warping
Modelling of nucleation and grain growth prediction	Phase-field model	Numerical simulation of microstructure evolution and properties by an order parameter based on free energy.	Microstructure evolution [93,99], nucleation [100].

A more accurate model requires transient analysis, consisting of fully coupled arc physics, heat and mass transfer, and stress evolution. In order to manufacture components of high quality by this arc-based AM process, optimization of process parameters and deposition strategy by several experimental trials and errors leads to an expensive and time-consuming process. To evaluate, some of the common defects of the WAAM process are residual stress, distortion, delamination, and surface roughness which have a significant impact on the properties and functionality of the manufactured part. Apart from the RP process parameters wire composition also affect the residual stresses and resulting microstructure in additively manufactured part. Along with these defects, we also need to predict different grain morphologies, crystallographic orientation, and grain size distribution with respect to the function of positioning, for which numerical modeling tools play a significant role. Hence, there will be a requirement for developing a computational tool for the wire-based DED. Process, which will facilitate the online inspection of components without destroying the AM part.

2.5.1 Heat transfer model for wire arc additive manufacturing process

Rapid heating, melting, cooling, and solidification of different regions of a fabricated component resulting from its interaction with a moving heat source leads to the development of multiple thermal cycles in a previously deposited layer. Continuous moving of the heat source and the temperature changes during deposition of material provides the transient temperature and others key variable which affect the quality of the part. It is not possible to measure the temperature directly during deposition (or) between the successive layers by

utilizing any contact technologies. Hence, in order to overcome these difficulties, there is a need for the development of a numerical heat transfer model. The deposition process will be simulated using a three-dimensional numerical model developed by Ding et al. [101] using an element and birth technique. This implies the elements to be activated sequentially, following the motion of the heat source as the material is deposited. Element birth technique used for deposition via user subroutine has the following advantages.

- There are no errors or ill-conditioning introduced by scaling factors, as is the case of the quiet element method.
- Element residual and Jacobian calculations are performed for active elements only.
- Only the active nodal degrees of freedom are considered at a time resulting in smaller algebraic systems by the Newton– Raphson linearization.

2.5.2 Mathematical representation of heat sources

An enumerative depiction of the energy distribution of the heat source is necessary for the exact computation of heat transfer, solidification, deposit's geometry, and its structure and properties. Their mathematical descriptions vary, and they can be broadly categorized as a point source, line source, power distributed over an area (i.e., surface heat flux), and power distributed over a volume (volumetric or body heat flux). Point and line heat source commonly used in analytical solution of conduction equation whereas surface and body heat flux are exclusively used in numerical simulation of heat transfer and fluid flow in AM process.

2.5.3 Heat sources for wire-based DED process

In the DED-GMA process, the filler wire absorbs heat in a manner similar to that for a consumable electrode in fusion welding processes. The wire is sometimes preheated by resistive or inductive heating or using a secondary heat source to enhance heat input and increase melting rate. A volumetric heat source is normally used to simulate the DED-GMA process [102]. The double ellipsoidal asymmetric distribution of power density of the heat source [103] was used to apply the heat to deposit in AM process, as shown in Figure 2.4. Fusion zone forms in AM generally display a tear drop shape because of the motion of the heat source and the flow of liquid metal within the molten pool. Mathematical expression for this

volumetric heat source model for the region in front of the arc and the region behind the arc center is given by:

$$q_f(x, y, z) = \frac{6\sqrt{3}(f_f\eta Q)}{\pi\sqrt{\pi}a_fb c} \exp\left[-3\left(\frac{x^2}{a_f^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}\right)\right] \quad (2.6)$$

$$q_r(x, y, z) = \frac{6\sqrt{3}(f_r\eta Q)}{\pi\sqrt{\pi}a_fb c} \exp\left[-3\left(\frac{x^2}{a_r^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}\right)\right] \quad (2.7)$$

$$f_f + f_r = 2 \quad (2.8)$$

where a_f and a_r are the length of the front and rear ellipsoid, b is the width of heat source, c is the depth of the heat source, Q is the heat energy input, η is the factor of efficiency, f_f and f_r are the factors for distributing the power to the front and rear of the heat source.

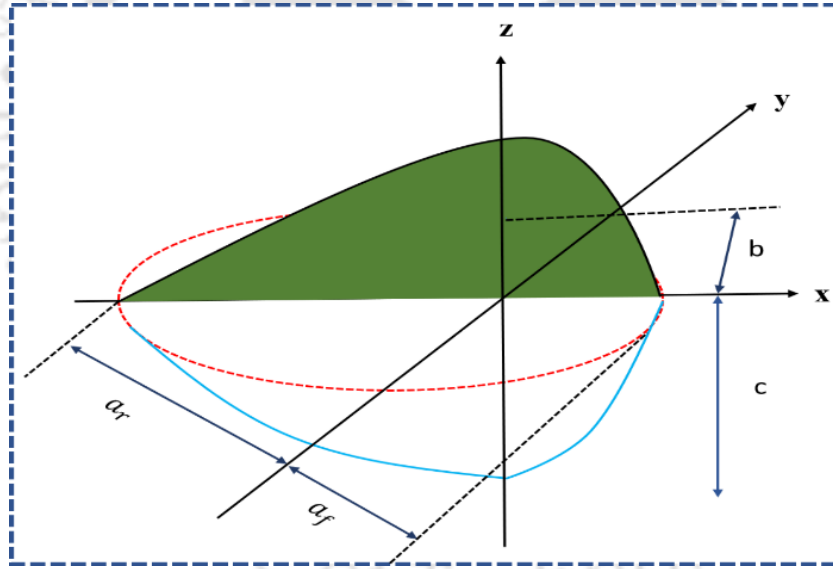


Figure 2.4: Schematic diagram of double ellipsoidal heat source [104].

In AM process, parts are manufactured by adding material layer by layer, due to which repeated heating, melting, cooling, and solidification takes place across different regions of additively manufactured parts by interacting with a moving heat source, which will develop multiple thermal cycles at any point. Commonly used techniques for the modeling of metal deposition in heat transfer analysis both quiet and inactive element activation is the finite

element method for the DED Process [105]. Ding et al. [101] developed a thermomechanical model of WAAM process wire using finite element-based commercial code software ABAQUS. However, different parameters varying during deposition have a significant impact on the variation of geometry, leading to the violation of the assumption of the flat bead and was found to influence both thermal and mechanical analysis during the DED process. Hence, Walker et al. [106] and Bailey et al. [107] developed a novel numerical model which considers the transient geometry and surface profile of deposited material, and its impact on the thermal and mechanical analysis was considered for DED. based AM process. By considering the moving heat source model, precise measurement of transient temperature and other important AM variables which are required for the computation of residual stresses, distortion, grain morphology, fusion zone geometry, and texture are determined. Heat transfer phenomena in AM largely depend on the geometry of the heat source model. Different geometrical features of heat sources like point, line, area, and volume affect the thermal cycles, solidification parameters; hence it is essential to develop a correct heat transfer model which will be able to consider all these variations and be used as a standard numerical tool for the spatial variation of microstructural and mechanical properties in the additively manufactured component.

2.6 Solid-state phase transformations in the additive manufacturing process

When the deposited material is solidified and cools below solidus temperature to room temperature, hence solid-state phase transformation occurs [108]. However, this phase transformation occurs at a lower temperature transforms back to a higher temperature phase due to cyclic heating during the deposition of material which alters the residual stress and distortion of additively manufactured components [37,109].

2.6.1 Phase transformation in steel

During heating and cooling cycle, steels experiences a series of phase transformation like for low alloy steels are α –ferrite to γ -austenite, δ -ferrite to liquid, and δ -ferrite to γ -austenite [110]. Microstructure of steel additively manufactured part was found to vary along build height direction due to variable cooling rate as for layer which was already deposited experiences a post-heating and the layer which need to deposit undergoes pre-heating. Jinguo et al. found in their study that martensite content increased gradually from the 5th layer to the

25th layers, indicating that metastable martensite partly decomposed into stable ferrite due to the carbon atoms diffusion [111]. Model for Solid-state phase transformation in steels has been developed based on thermodynamic and kinetic principles. Necessary input data required by the model include the chemical composition, the prior austenite grain size, and the cooling curve. The volume fractions of allotriomorphic ferrite, Widmanstätten ferrite, acicular ferrite, and martensite can be computed as the output of these models [112]. Isothermal time-temperature-transformation (TTT) and continuous-cooling-transformation (CCT) diagrams calculated by phase transformation models provide tools to calculate the final phase fraction due to transient heating [113].

2.7 Finite element based numerical modeling for AM process

Numerical modeling and simulation techniques using FE methods are used as a standard tool to quantify the common defects of the WAAM process, which allows the researcher to control the several AM process parameters to make part defect-free, sound mechanical properties, and high reliability. Finite element-based numerical analysis is generally used for thermomechanical analysis and topology optimization for AM process. Fabrication of components by AM technique consists of layer-by-layer process; hence, it is impossible to measure temperature during processing or finished product directly or by using any contact technologies. Manvatkar et al. [114,115] developed a novel three-dimensional numerical heat transfer model using a finite element tool to predict the temperature field and layer profile for a single bead and multi-layer during the deposition of H13 tool steel for powder-based DED technique using laser as a heat source for melting as shown in Figure 2.5. In order to do the thermal and mechanical analysis of the deposited layer, Finite element (FE) based numerical analysis is used to predict the variation of temperature along with increasing height and deformation in the WAAM process [116]. In some of the studies by coupling the FE-based numerical modeling and thermo-mechanical-metallurgical(TMM) model to know the effect of solid-state phase transformation kinetics (SSPT) on residual stresses (RS) analysis were done for AM process [117–119].

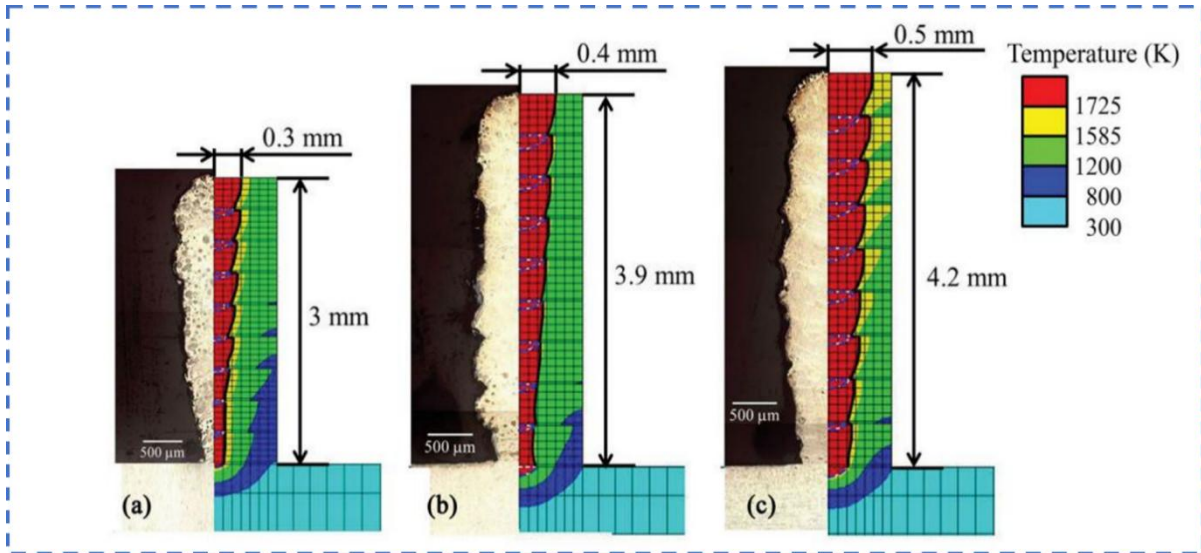


Figure 2.5: Comparison of actual deposited profile experimentally (left) and computed (right) of a single bead of (a) third (b) fifth and (c) nine layers by the varying process during powder-based DED technique using laser as a heat source [115].

Idle time between successive layers also has a significant effect on inter-pass temperature during the deposition of material which prevents the occurrence of the collapse of a manufactured workpiece. Hence, the finite element-based numerical modeling of material deposition was used to optimize idle time between layers [120]. For FE-based analysis of arc-based RP processes, commonly used heat source models are Gaussian or Double ellipsoidal volumetric heat source consists of a number of meshes, making analysis time-consuming and expensive. A newly proposed well distributed volumetric heat source model is insensitive to mesh for the WAAM process; around 97% saving in computational time was found [36]. Till now, FEM has successfully been implemented in additive manufacturing industries for thermomechanical analysis of fabricated components, as shown in Table 2.3.

Table 2.3: Different FE-based thermomechanical models for simulating additively manufactured parts.

Additive manufacturing process	Deposited Material	Software utilizes for simulation	Simulation description	Ref.
DED-L	H13 tool steel	ABAQUS	Rectangular block with 55,455 elements and 60,033 nodes	[121]
PBF-L	Ni-Ti shape memory alloy	ANSYS	Rectangular block with brick elements	[122]
	Ti-6Al-4V	COMSOL	Impeller with complex geometry	[123]
PBF-EB	IN718	ABAQUS	Rectangular component with multiple layers and multiple hatches	[124]
	Ti-6Al-4V	ABAQUS	Blocks with support structures and overhang	[125]
DED-GMA	Low carbon steel	ANSYS	Rectangular block with multiple layers	[126]
	S355JR-AR	ABAQUS	Single bead multi-layer deposit	[101]

2.8 Residual stress and distortion in wire-based DED process

Due to rapid heating, melting, solidification, and cooling of the part during the fabrication of component by AM process in a layer-by-layer fashion. Different locations of the part manufactured experience repeated heating and cooling cycles which leads to develop complex

stresses and strains as it originates from restricted thermal expansion and contraction [1,127]. The magnitude of developed residual stress and distortion depends on the geometry of the part[106], deposition geometry [107], material properties [128], process parameters [129], scanning strategy [81,130], substrate preheating temperature [69], substrate design [131], a clamping strategy used for restricting the degree of freedom(DOF) [132], and also a solid-state phase transformations [133–136] like a transformation of austenite to ferrite in steels having a significant impact. If these induced residual stresses inside the component exceed the yield strength of the material may cause delamination, buckling, warping, and it also diminishes down the fatigue life of the components [90]. If the dimension of the additively manufactured component is not within the specified limit due to distortion, then it leads to the rejection of the part. Hence, a reckonable understanding of the development of residual stress due to transient temperature variation is required to control or mitigate the above-mentioned issues.

2.8.1 Thermomechanical model to calculate residual stresses and distortion in WAAM process

A finite element-based thermomechanical model is generally used to evaluate the variation of temperature with time and residual stress distribution in 3D. This model first calculates the transient temperature distribution by the numerical solution of the heat conduction equation. Obtained temperature field (thermal load) is then transferred to the mechanical model for stress analysis. The thermomechanical model computes residual stresses by evaluating total strain increment with the variation of time during the WAAM process [137]. An increment of total strain is given by:

$$\Delta \varepsilon_{ij}^{total} = \Delta \varepsilon_{ij}^e + \Delta \varepsilon_{ij}^{th} + \Delta \varepsilon_{ij}^p + \Delta \varepsilon_{ij}^v \quad (2.9)$$

where $\Delta \varepsilon_{ij}^e$, $\Delta \varepsilon_{ij}^{th}$, $\Delta \varepsilon_{ij}^p$ and $\Delta \varepsilon_{ij}^v$ are the elastic, thermal strain increment, plastic, and strain developed due to solid-state phase transformation. Stress developed from the elastic strain is given by[138]:

$$\Delta \sigma_{ij}^E = D_{ijlm} \Delta \varepsilon_{lm}^E \quad (2.10)$$

where D_{ijlm} is the elastic stiffness matrix evaluated from the modulus of elasticity (E) and Poisson's ratio μ as given by Hooke's law:

$$D_{ijlm} = \frac{E}{1+\mu} \left[\frac{1}{2} (\delta_{il}\delta_{jm} + \delta_{lm}\delta_{ij}) + \frac{\mu}{1-2\mu} \delta_{ij}\delta_{lm} \right] \quad (2.11)$$

where $\delta_{ij}, \delta_{il}, \delta_{jm}, \delta_{lm}$ are Kronecker delta whose value is unity for $i=j$ else it's zero for $i \neq j$. To consider the temperature dependent plasticity according to Von Mises yield criteria is used to simulate flow stress and plastic strain. Strain developed due to transient temperature field is given as:

$$\Delta \varepsilon_{lm}^{th} = \alpha \Delta T \quad (2.12)$$

where α is the coefficient of thermal expansion and ΔT is a transient temperature increment.

2.8.2 Residual stress and distortion developed for single alloy components

Residual stress and distortion developed inside the fabricated part are spatially non-uniform depending on the transient temperature field, geometric constraints, and temperature-dependent mechanical properties. The above-mentioned thermomechanical model is used for simulating the evolution of residual stress during the WAAM process. Figure 2.6 illustrates the thermomechanical simulation of wire-based DED and demonstrates how the time-varying thermal field governs residual stress and distortion. Figure 2.6a depicts the transient temperature distribution during layer-by-layer deposition, highlighting steep cooling gradients at the substrate–deposit interface and along the build height. Figure 2.6b shows the corresponding residual stress field for a four-layer steel wall in two states: as-fabricated (clamped) and after clamp release. During cooling, constrained thermal contraction concentrates tensile stresses within the deposited material while the cooler substrate sustains compensating compression; upon fixture removal, partial relaxation and spring-back redistribute these stresses and expose the distortion previously restrained by clamping. Overall, the figure demonstrates that the spatially non-uniform stress pattern arises directly from the transient temperature field under geometric constraint and temperature-dependent material response captured by the model.

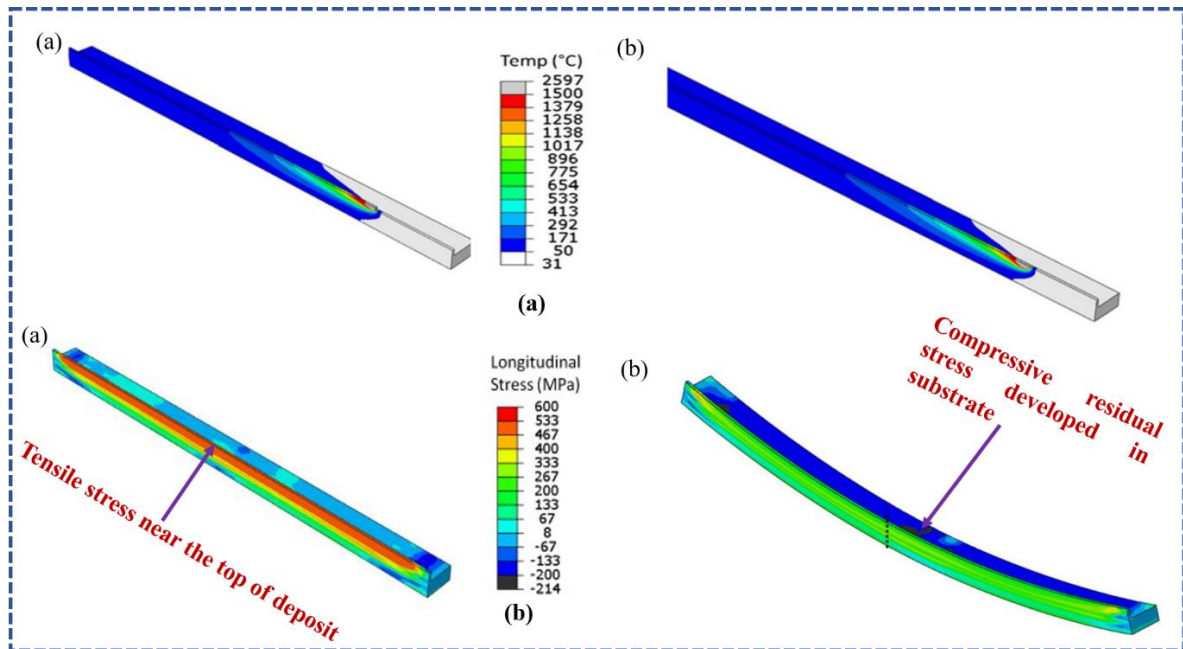


Figure 2.6: Numerical model for the deposition of material in wire-based DED. (a) Transient temperature distribution (b) Residual stress distribution during four-layer structure steel deposit as printed and after releasing the clamp [101].

2.8.3 Residual stress and distortion in functionally graded alloys

The variations in thermo-physical and mechanical properties present two challenges for controlling residual stress and distortion in functionally graded alloys. Residual stress evolves during the cooling of a component because the alloy contracts as it cools but is restrained by neighboring material or mechanical clamps attached to the build plate. In a single alloy, the extent and rate of contraction are largely governed by the spatial variation cooling rates and temperature gradients during the cooling process. In a functionally graded part, differences in thermal expansion coefficients can lead to the development of unique residual stresses and distortion patterns. Variations in thermo-physical properties can also lead to different cooling rates and temperature gradients during cooling, further influencing the development of residual stresses [139]. However, the yield strength varying significantly in the graded component of different materials; hence there will be a probability that two different regions having the same magnitude of residual stress but are sensitive to different values of delamination, buckling, and warping. Zhang et al. [140] developed a thermomechanical model of FGMs between H13 tool

steel and Cu. The failure between these materials was mitigated by introducing interlayers of nickel-based superalloy (D22) as shown in the below Figure 2.7.

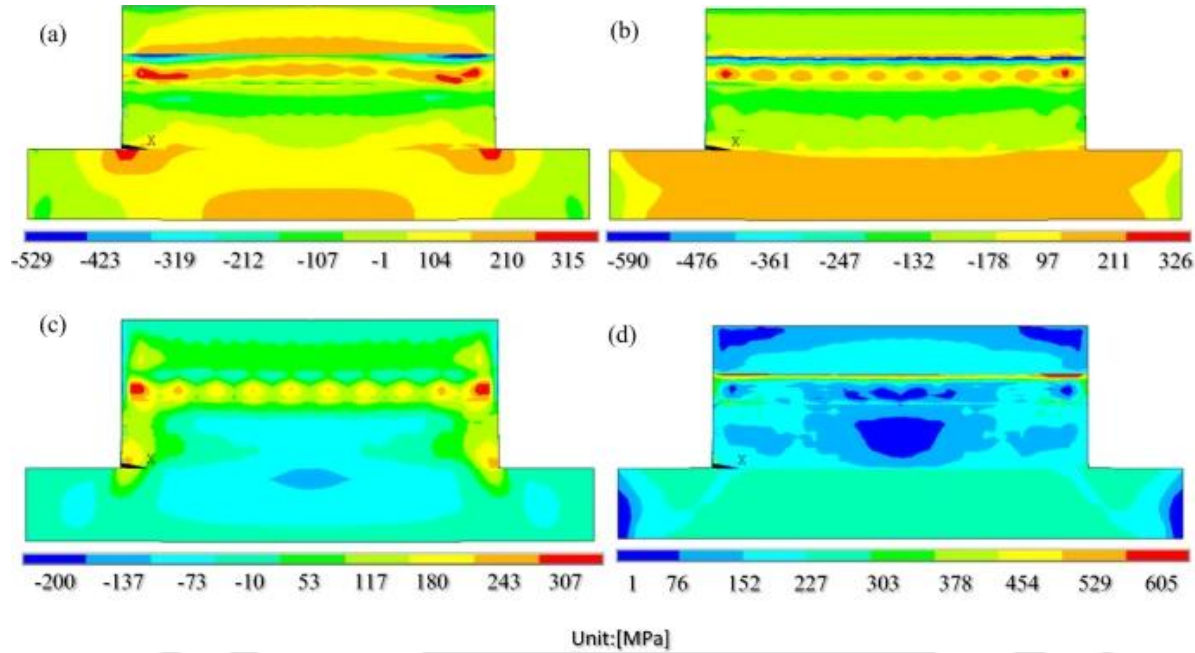


Figure 2.7: Longitudinal residual stress σ_{11} observed from (a) side and (b) middle (c) through-thickness stress σ_{33} and (d) von misses stress of the CuD22H13 after deposition [140].

2.9 AI driven thermo-mechanical model

Artificial Intelligence (AI) serves as the broad umbrella encompassing technologies that emulate human intelligence to perform complex tasks such as reasoning, decision-making, and learning. Within AI, Machine Learning (ML) emerges as a data-driven approach that enables systems to identify patterns and make predictions by learning from historical data, without explicit programming for each task. Deep Learning (DL), a specialized subset of ML, leverages multilayered neural networks to automatically extract hierarchical features from vast and unstructured datasets, offering superior capabilities for high-dimensional and nonlinear problems. In the context of arc-based DED, this hierarchical framework (AI > ML > DL) plays a pivotal role in predicting and controlling deposition characteristics such as bead geometry, thermal field evolution, and residual stress distribution. While traditional numerical and experimental techniques struggle with scalability and real-time adaptability, AI models efficiently analyze complex interactions among deposition parameters and rapidly infer

optimal conditions. ML techniques like decision trees and support vector machines can identify key process drivers affecting bead morphology or porosity, while DL models can decode intricate thermal patterns from in-situ images to forecast melt pool behavior or stress accumulation. Together, these AI-driven approaches provide an intelligent, scalable, and interpretable solution for optimizing deposition quality and enabling closed-loop control in arc-based DED. In context of arc-based DED, the prediction and control of key deposition characteristics, such as bead geometry, thermal profile evolution, and residual stress accumulation are essential for ensuring structural integrity, dimensional precision, and repeatable quality in manufactured components. However, these characteristics are governed by complex, non-linear interactions among multiple thermal, mechanical, and metallurgical variables, including arc power, deposition speed, substrate preheat temperature, thermal conductivity, and solidification behaviours.

Traditional experimental methods, although accurate, are often constrained by the need for extensive instrumentation and are unable to provide continuous in-situ insights due to the harsh thermal environment inherent in high-temperature metal additive processes. Numerical techniques based on FE methods, while useful in capturing the underlying physics by solving conservation equations and constitutive models, require significant computational resources. These models often involve long simulation times ranging from hours to days depending on geometry, material complexity, and boundary condition definitions, which makes them unsuitable for rapid process exploration or real-time control. To address these challenges, the deployment of artificial AI, particularly PIML models, offers a highly efficient and scalable alternative. These models are capable of learning intricate relationships between deposition parameters and output characteristics without solving complex partial differential equations. By embedding physics-based variables such as cooling rate, temperature gradient to solidification rate ratio (G/R), and solidification-induced stress into the learning process, physics-informed ML frameworks bridge the gap between black-box data-driven predictions and physically grounded interpretation. Deep learning models like neural networks, when trained on thermal imaging, simulation, or sensor data, can accurately forecast temperature evolution, melt pool behaviours, and residual stress fields, even in dynamically changing deposition scenarios. Furthermore, ensemble methods such as random forests and gradient-boosted trees can reveal the hierarchy of process parameter importance, helping identify which

inputs most strongly influence defects like cracking, warping, or dimensional distortion.

The integration of AI into DED modelling pipelines is further empowered by powerful libraries such as Scikit-learn, TensorFlow, and Keras, which facilitate rapid model development, hyperparameter optimization, and deployment. These tools enable researchers to transition from large, time-consuming design-of-experiment (DOE) frameworks such as the 2-factor DOE for crack causation that would traditionally require thousands of runs to compact, high-fidelity AI models capable of delivering equivalent insights with a fraction of the computational or experimental burden. Moreover, AI models excel in capturing multi-variable correlations and real-time adaptive behaviours, making them suitable for predictive digital twins and closed-loop control architectures. These capabilities are particularly valuable in identifying defect root causes, optimizing process windows, and accelerating qualification cycles for new materials and geometries. In conclusion, AI offers a paradigm shift in the prediction of deposition characteristics in arc-based DED. By combining data-driven modelling with physics-informed insights, AI enables faster, more interpretable, and scalable solutions for understanding and optimizing additive manufacturing processes. As the field advances toward autonomous, quality-assured fabrication, the integration of AI will be pivotal in driving intelligent control, minimizing defects, and elevating the overall reliability of metal additive manufacturing.

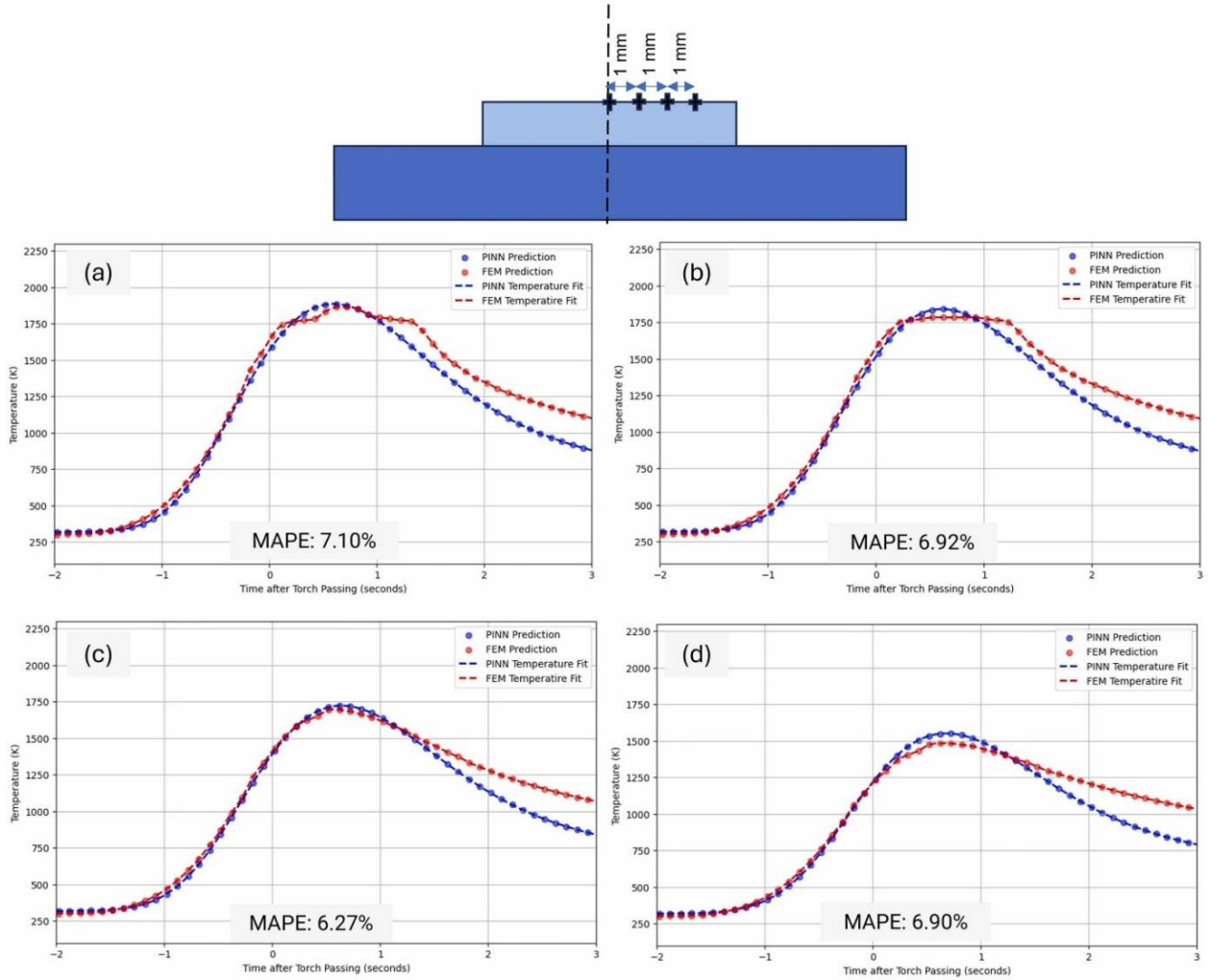


Figure 2.8: Temperature evolution comparison between the low-fidelity PINN model and FEM simulation at multiple surface locations across the bead cross-section: (a) bead centerline, (b) 1 mm offset from center, (c) 2 mm offset, and (d) 3 mm offset, illustrating spatial prediction accuracy [141].

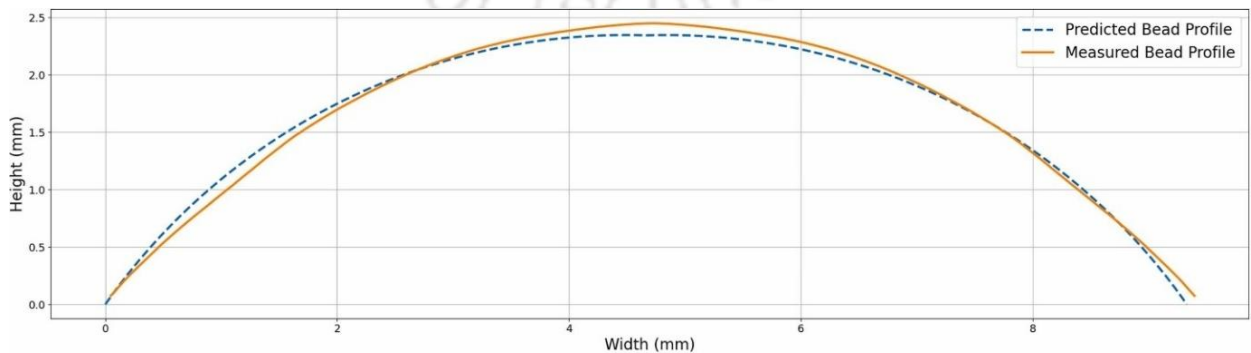


Figure 2.9: Comparison between predicted and experimentally measured bead geometries obtained using the low-fidelity PINN model, demonstrating its effectiveness in capturing profile accuracy [141].

Rashid et al. [141] presents a physics-informed neural network (PINN) framework for predicting bead geometry in arc-based DED, a metal additive manufacturing process where traditional numerical simulations and purely data-driven models often fall short in balancing accuracy and computational efficiency. By coupling a thermal model with a geometric predictor, the PINN framework captures the complex thermo-geometric interactions inherent to the process (Figure 2.8 and 9). Two variants, a high-fidelity model with fine spatiotemporal resolution and a low-fidelity model with coarser resolution are evaluated. While the high-fidelity PINN achieves slightly better accuracy (8.38% height error, 1.09% width error), the low-fidelity version delivers comparable results (8.33% height error, 1.56% width error) with a 79% reduction in training time and significantly lower computational cost. Incorporating minimal experimental geometry data further enhances model precision. The framework demonstrates robust generalization across different deposition locations, establishing it as an efficient and scalable solution for real-time bead geometry. Zamiela et al. [142] introduces a physics-informed, multi-sensor data fusion framework to predict surface deformation in arc-based DED by reconstructing internal thermal histories. Addressing the limitations of individual in-situ thermal sensors such as limited field of view and spectral range, this approach integrates infrared (IR) thermal data with a physics-based Goldak double ellipsoidal heat flux model to estimate internal heat input. This fused data informs a physics-informed model input (PIMI), which accurately approximates the internal thermal field. A regression-based convolutional neural network (CNN) is then used to correlate the reconstructed 3D thermal gradients with resulting surface deformation. Applied to thin-walled AM structures, the model achieves a mean squared error of 1.14 mm and an R^2 value of 0.89, demonstrating its potential for real-time quality monitoring and deformation.

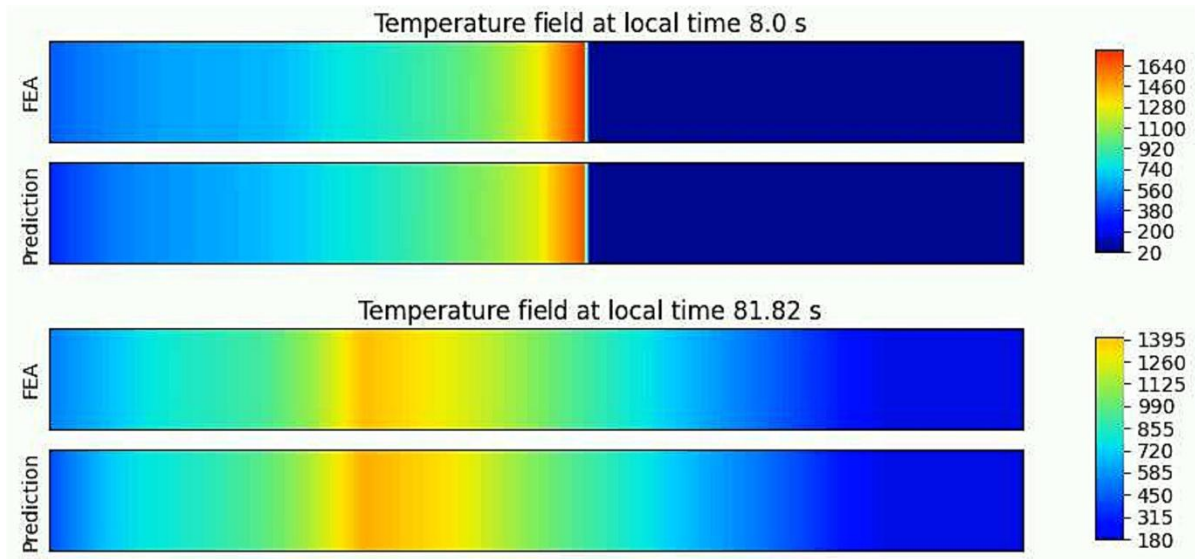


Figure 2.10: Comparison of predicted and simulated thermal fields at the 20th deposition layer under varying process parameters, highlighting the model's validation accuracy across different conditions [143].

On advancement of above Tang et al. [143] study introduces a real-time thermal field prediction framework for DED of thin-walled structures, targeting practical challenges in online process control with minimal sensor input (Figure 2.10). The proposed method employs a two-stage approach: first, artificial neural network maps temperature curve segments from previously printed layers to estimate the thermal profiles of yet-to-be-printed regions; second, a reduced-order model (ROM), trained using an extreme learning machine (ELM), reconstructs the full-layer thermal field from a few known temperature profiles. Validated through 15 physical WAAM experiments and 9 simulations, the model predicts layer-wise thermal fields within 0.1 seconds on a standard desktop CPU. It demonstrates strong generalization across varying layers and printing conditions, and after minimal fine-tuning, achieves low relative error in unseen experiments.

Moving towards the prediction of thermos-mechanical responses, Wu et al. [69] presented a pioneering study that integrates thermomechanical modeling with machine learning to uncover the hierarchy of variables governing residual stresses in WAAM. By analyzing 243 datasets across IN718, SS316, and 800H alloys using neural networks and random forests, they achieved more than 97% predictive accuracy (Figure 2.12) and identified substrate preheat

temperature as the most critical process parameter, followed by arc power, substrate thickness, and scanning speed (Figure 2.11). More importantly, they established five composite thermomechanical variables: solidus to preheat temperature gap, stress per unit temperature change, molten pool volume, substrate rigidity, and heat input. Among these, the temperature gap emerged as the dominant factor since stresses primarily form during cooling through this range. Their process maps provide practical guidelines to mitigate delamination, highlighting how data driven approaches can accelerate parameter optimization and enable defect free WAAM components. Further, Zhou et al. [144] presents an evolution-based tool-path planning strategy to enhance thermo-mechanical properties in arc-DED. While continuous tool paths improve deposition efficiency, the clustering of adjacent paths often leads to poor thermal regulation and mechanical performance. To address this, the authors develop a genetic algorithm tailored to the deposition context, incorporating customized crossover and mutation operations. A fast thermo-mechanical field prediction model enables rapid fitness evaluation within seconds, significantly reducing the planning time. Moreover, a formability constraint ensures that the generated paths maintain part quality. Experimental results show that the optimized toolpaths improve thermo-mechanical performance by over 87% and reduce residual von Mises stress by more than 32 MPa. The proposed method achieves these gains within a practical planning time frame of roughly one hour, offering a substantial improvement over conventional numerical simulations that require several hours per evaluation.

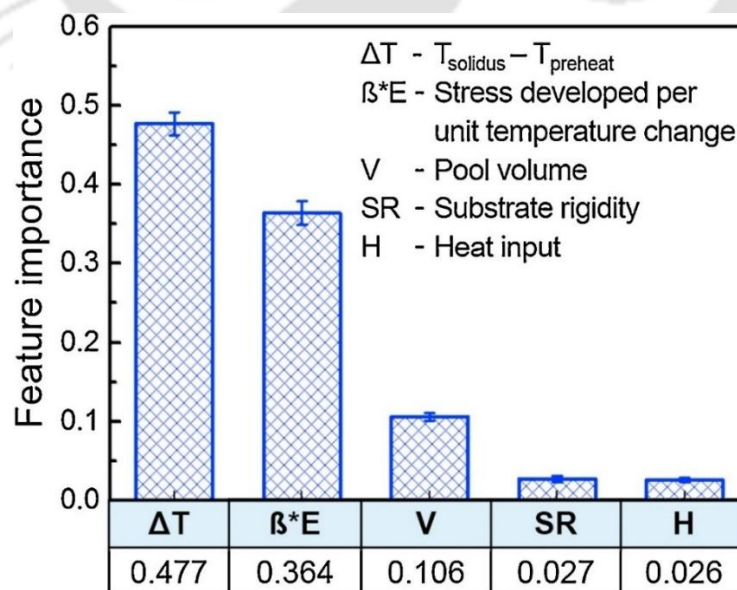


Figure 2.11: Feature importance of the causative parameters as determined by the random forest model [69].

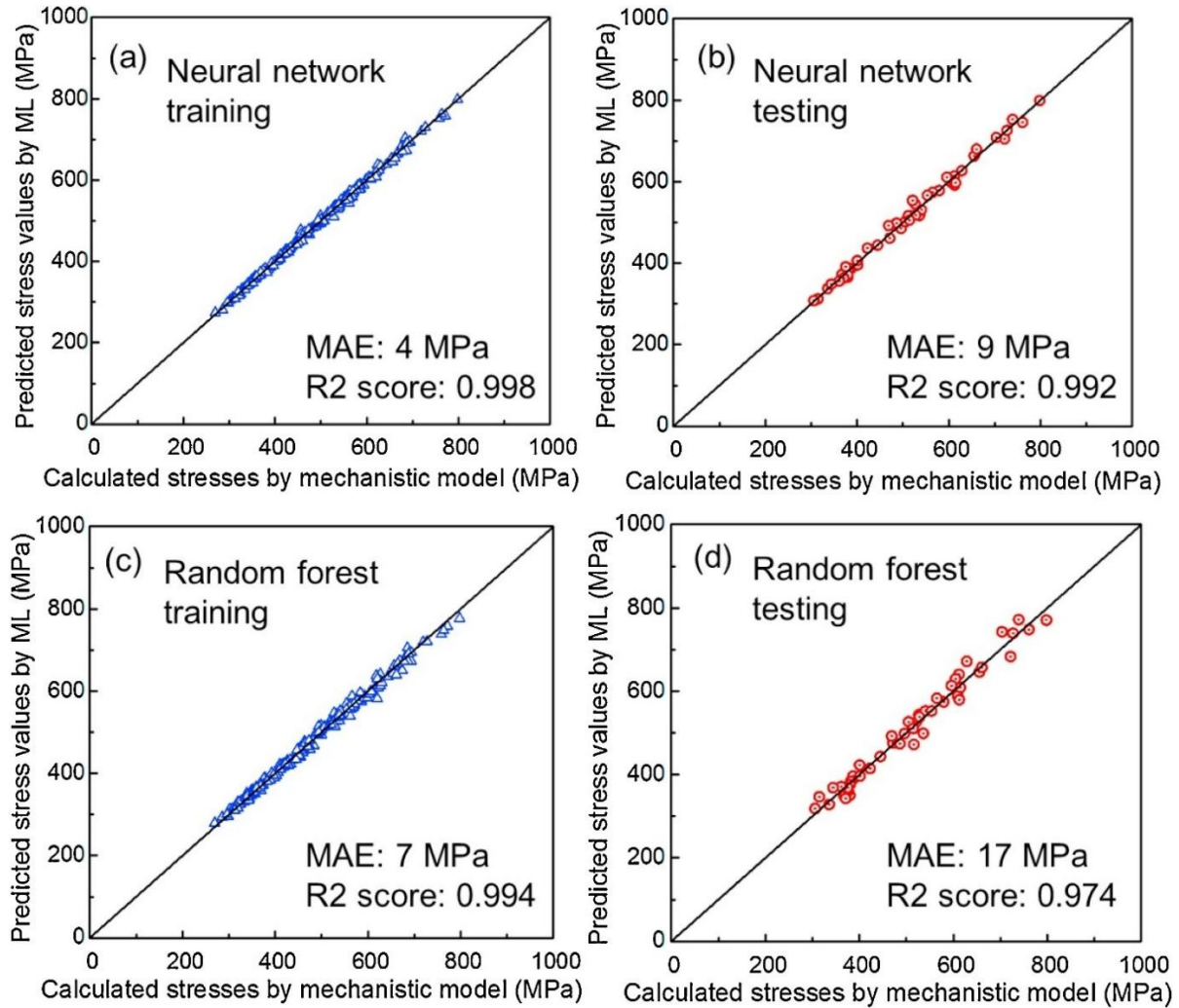


Figure 2.12: Comparison of residual stress predictions and thermomechanical model results for WAAM: (a, b) training and testing datasets using the neural network with five complex thermomechanical variables, and (c, d) training and testing datasets using the random forest model with the same variables [69].

In pursuit of a real-time digital twin (DT) for metallic additive manufacturing, this study presents an adaptive online distortion simulation framework tailored for arc-DED. Overcoming the limitations of traditional numerical simulations and conventional data-driven models, the approach employs a hybrid generative machine learning architecture. It integrates

a Vector Quantized Variational AutoEncoder with a Generative Adversarial Network (VQVAE-GAN) for extracting spatial features of distortion, while a Recurrent Neural Network (RNN) fuses temporal dynamics by Mu et al. [145]. Pretrained offline using FEM distortion data and executed online with laser-scanned point clouds during deposition, the model accurately predicts evolving distortion fields in real time (Figure 2.13). Experimental tests on seven thin-walled structures validate their robustness, achieving a root mean square error (RMSE) below 0.9 mm significantly outperforming FEM and ANN-based methods by 143% and 151%, respectively. This advancement marks a major step toward implementing real-time, AI-driven digital twins in metallic AM environments.

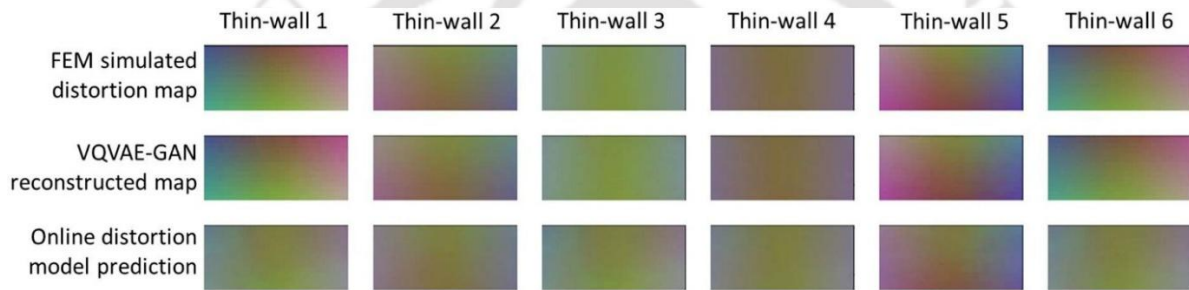


Figure 2.13: Comparison of FEM-based distortion maps reconstructed latent features from the VQVAE-GAN model and predicted distortion outputs from the proposed online simulation framework at the 20th deposition layer for each case [145].

In order to capture the thermo-mechanical responses of multi-track-multi-layer deposits, Sharma et al. [146] paper demonstrates a clean bridge between high-fidelity FE simulation and physics-informed neural networks (PINNs) (Figure 2.14). The authors benchmark a FE model and then design a thermo-mechanical PINN that separates temperature and stress/displacement networks, directly outputting the six stress components to avoid per-iteration constitutive back-calculations. Crucially for parametric studies, transfer learning from a base model (500 W, 10 mm/s) enables rapid adaptation to new power/speed pairs in minutes while retaining temperature accuracy stress fidelity remains best when the source model is pre-trained at the highest energy density. The present framework is thermoelastic with constant properties (no latent heat, fluid flow, or plasticity), so long-horizon accuracy decays after ~ 0.8 s without refresh; a practical takeaway for a digital-twin workflow is to couple PINN inference with

sparse FE “refresh” windows around expected peak-stress times and, for realism, extend the physics to temperature-dependent properties, phase change, and elastic-plastic response. Overall, this is a strong template: use FE once to set physics, mesh/BCs, and targeted labels; use a two-network thermo-mechanical PINN with stress outputs and adaptive collocation for fast, transferable stress prediction across process windows.

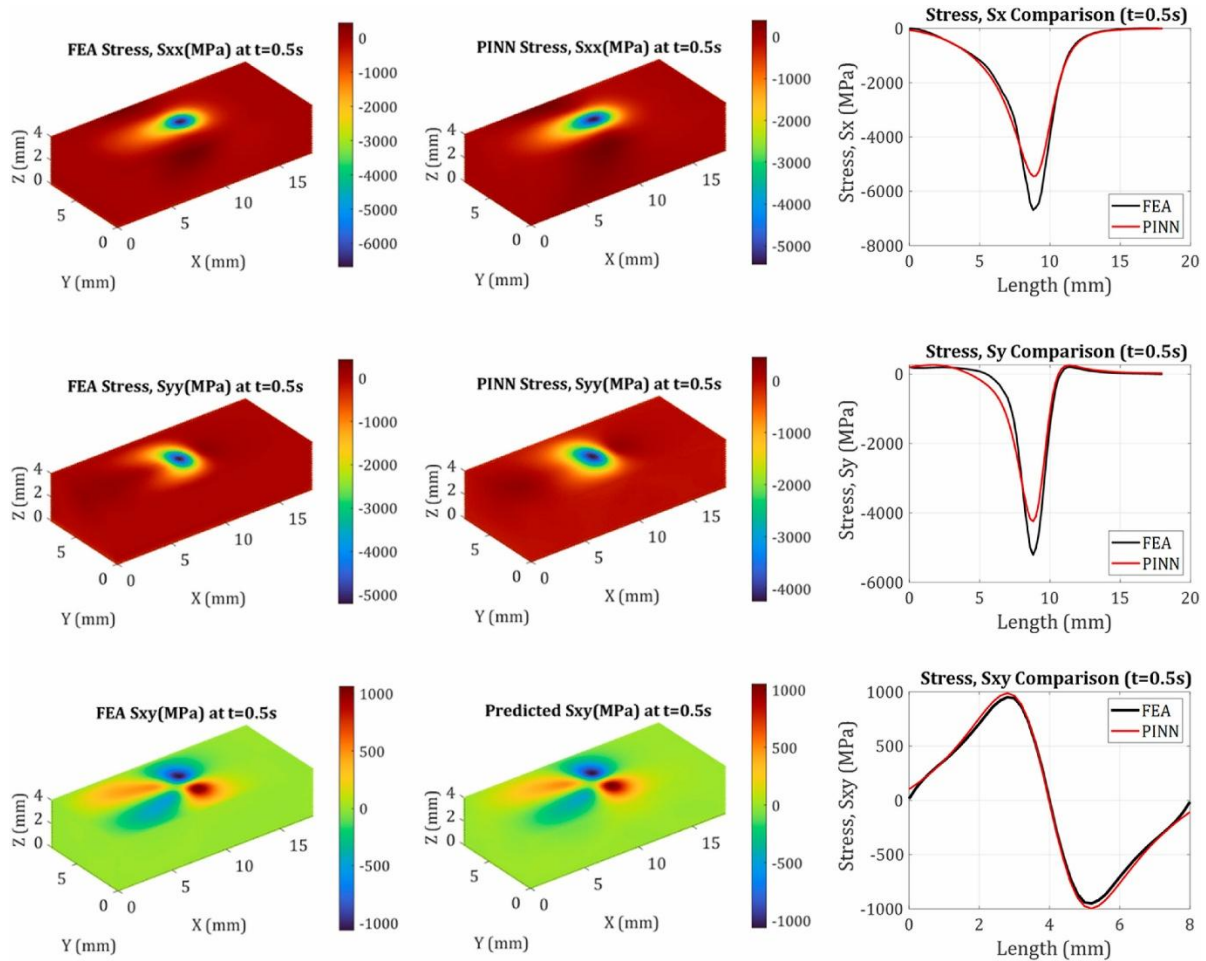


Figure 2.14: Comparison of stress distributions obtained from (a) finite element analysis, (b) physics-informed neural network predictions, and (c) top-surface profile extracted along the central line [146].

2.9 Summary

Available literature depicts that AM combined with data science provides a pathway for predictive control of process and performance, particularly in wire-based DED, where transient

thermal cycles govern microstructure and residual stress evolution. Direct measurement of melt pool temperature is limited, as infrared cameras cannot capture moving tracks and thermocouples suffer time lag, making physics-based FE models the preferred option. While accurate, these simulations are computationally demanding due to nonlinear interactions among process variables, motivating the integration of ML to extract correlations and accelerate predictions. Traditional ML methods such as DT, RF, XGBOOST, and ANNs capture nonlinear relationships but struggle with sequential data. RNNs including long short-term LSTM and GRU, and more recently TCNs, overcome this limitation by encoding temporal dependencies, enabling accurate prediction of layer-wise thermal and stress histories. When trained with physics-based features from validated FE models, these algorithms form physics-informed ML frameworks that preserve mechanistic fidelity while reducing computational cost, often achieving near-FE accuracy with orders-of-magnitude faster execution.

Among WAAM variants, GMAW provides high throughput but suffers from arc instability and oversized molten pools, while CMT offers superior arc stability, minimal spatter, and refined microstructures due to higher cooling rates. Although CMT-based WAAM has been applied to a wide range of alloys including aluminum, titanium, steels, and nickel-based superalloys, much of the existing work remains observational, with limited mechanistic insight into how thermal cycles, cooling rates, and scanning strategies govern anisotropic microstructure development and residual stress evolution. The generation of tensile residual stresses in WAAM is fundamentally driven by steep thermal gradients and non-uniform cooling that arise during cyclic melting and solidification of successive layers. These stresses, if unmitigated, promote distortion, dimensional inaccuracy, and premature failure, particularly in creep-strengthened alloys such as 9Cr–1Mo steel where long-term mechanical reliability is critical. Although post-processing treatments such as normalization, tempering, homogenization, and aging remain effective for residual stress relief and microstructural refinement, their application is often impractical for large or complex geometries. Hence, research emphasis is shifting toward in-process optimization, particularly the control of inter-layer dwell time and inter-pass temperature, which govern the balance between thermal accumulation and fresh martensite formation, as well as the adoption of advanced scan strategies that distribute heat uniformly. These levers, when optimized in conjunction with AI

frameworks that embed physics features from FE models into DL surrogates, offer a computationally efficient and physically interpretable pathway to predict and tailor residual stress fields in WAAM-fabricated structures. Such integrated approaches not only minimize the risk of Type IV cracking in 9Cr–1Mo steels under high-temperature service but also provide a generalizable route for residual stress control in other AM alloys, thus advancing the broader vision of intelligent, data-driven additive manufacturing.

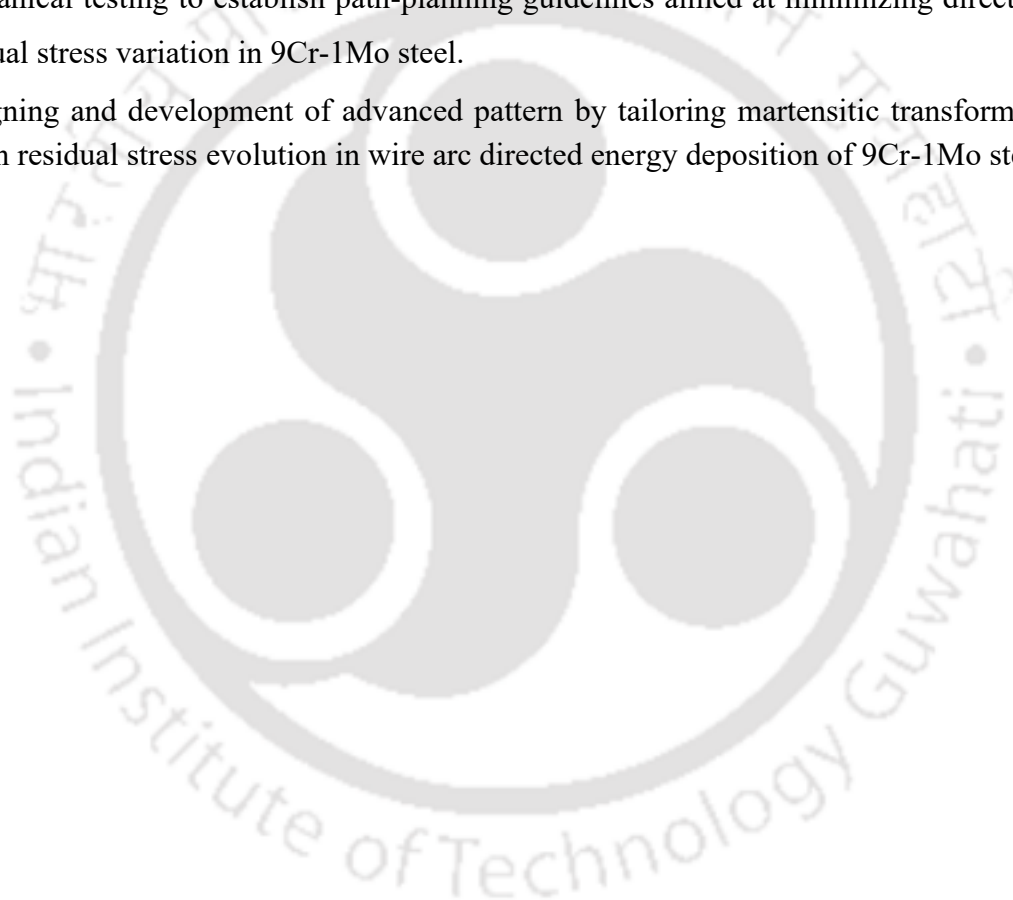
Scope of present work

The literature survey highlights key gaps in wire-based DED of 9Cr-1Mo, fast and generalizable thermal prediction remains limited. Residual-stress predictions rarely capture full ordinal nature of transient evolution. The quantitative role of inter-layer dwell time is under-resolved for ferritic steels, scan-path design is seldom linked rigorously to microstructure-stress co-evolution, and martensitic transformation is not yet exploited as a controllable lever for beneficial stress states. The scope of the present work is to tailor residual-stress evolution by tightly coupling experiments, FE based thermo-mechanical simulation, and physics-informed/artificial-intelligence models within a digital-twin workflow. The key elements are summarized below:

- There is a requirement for the development of physics-informed machine learning models that replace cumbersome in-situ thermometry with a calibrated high-fidelity FE thermal model to generate rich spatiotemporal temperature datasets. These data, anchored by targeted experiments are used to train machine-learning models that incorporate physics through constraints and features. Models that achieve high predictive accuracy on representative validation datasets are selected to provide precise and efficient predictions of transient temperature profiles in 9Cr-1Mo steel.
- There is a need to develop a thermo-mechanical FE baseline that incorporates elastic–plastic, temperature-dependent properties to generate time-series residual stress data under varying deposition conditions. The framework will compile inputs from local thermal histories and process parameters. While advanced temporal models will be implemented to determine the most effective approach for producing accurate and computationally efficient stress predictions in DED-fabricated components.
- There is a requirement for the development of deep learning models to analyze inter-layer

dwelt time and inter-pass temperature responses in thin-wall structures. Thermal and stress surrogates will be employed to map dwell settings to thermal and residual stress, distortion, and delamination risk, with validation carried out through targeted residual stress measurements on representative builds.

- There is a requirement to investigate unidirectional and bi-directional scanning strategies under varying heat input conditions for ferritic steel. Numerically derived thermal and stress responses obtained using the developed surrogates will guide the fabrication of thin wall structures. The printed components will be characterized by microstructures and mechanical testing to establish path-planning guidelines aimed at minimizing directional residual stress variation in 9Cr-1Mo steel.
- Designing and development of advanced pattern by tailoring martensitic transformation driven residual stress evolution in wire arc directed energy deposition of 9Cr-1Mo steel.



Chapter 3

Experimental Investigations

3.1 General background

The present chapter describes the experimental methodology adopted for the deposition of 9Cr-1Mo ferritic steel using a CMT-based DED system integrated with a robotic arm. The study begins with single-track depositions to establish baseline process stability and bead geometry, followed by single-track multi-layer fabrication to examine layer-wise thermal effects and microstructural evolution. Building upon this, multi-layer walls are fabricated using different scanning strategies, including uni-directional and bi-directional patterns, to assess their influence on thermal cycling and residual stress development. Subsequently, multi-track multi-layer components are printed to emulate realistic part geometries and to investigate cumulative effects of deposition strategy and process parameters. Surface residual stresses in all deposited samples are quantified using portable XRD employing $\sin^2\psi$ method. Microstructural characterization is performed on the printed specimens using a combination of SEM, XRD, EBSD, and TEM) enabling detailed assessment of phase constitution, grain morphology, and defect structures. Mechanical properties of printed parts are further evaluated through uniaxial tensile testing and Vickers microhardness measurements, thereby providing a comprehensive correlation between process strategy, microstructure, and mechanical response.

3.2 Single track deposition of 9cr-1Mo steel

Single-layer deposition trials are conducted using CMT-based DED process to evaluate the influence of process parameters on bead geometry for 9Cr–1Mo steel. Key geometric attributes including bead height, width, and penetration depth are analyzed to ensure full substrate fusion and geometric consistency, which are critical for multi-track, multi-layer fabrication (Figure 3.1). The filler wire used is ER90SB91 with a diameter of 1.2 mm, shielding gas is provided using a gas mixture of 80 % argon and 20 % Co₂ at a flow rate of 15 L/min, with a fixed torch standoff distance of 12 mm maintained between the torch and substrate to ensure arc stability and uniform deposition. The interdependence of current, voltage, and wire feed speed in the CMT process, referred to as the synergic line, plays a crucial role in maintaining arc behavior and deposition characteristics, and for this study, synergic line number is selected based on compatibility with the chosen filler wire and shielding gas composition. Among the trial combinations, five exhibited complete fusion with penetration depths exceeding 2 mm. The maximum penetration of 3.6 mm was obtained at 2.2 kW and 3.3 mm/s, although the corresponding bead width of 8.5 mm may lead to overlap issues in dense build strategies. A well-balanced bead geometry is achieved at 2.8 kW and 5.7 mm/s, providing 3.0 mm penetration, 3.0 mm height, and 8.0 mm width indicative of efficient arc energy utilization and consistent layer morphology (Figure 3.1g). Higher speed conditions, such as 3.2 kW at 9.2 mm/s, led to a shallower penetration of 2.2 mm and narrower bead width (5.9 mm), due to reduced energy density (Figure 3.1e). On the other hand, lower power–higher speed regimes, including 2.2 kW at 15.0 mm/s and 1.6 kW at 12.6 mm/s, produce limited penetration depths of 1.3 mm and 1.6 mm, respectively, with correspondingly narrow beads (Figure 3.1 a and f). These findings clearly demonstrate that increased power coupled with lower scan speed enhances heat input, facilitating deeper fusion and more stable bead formation.

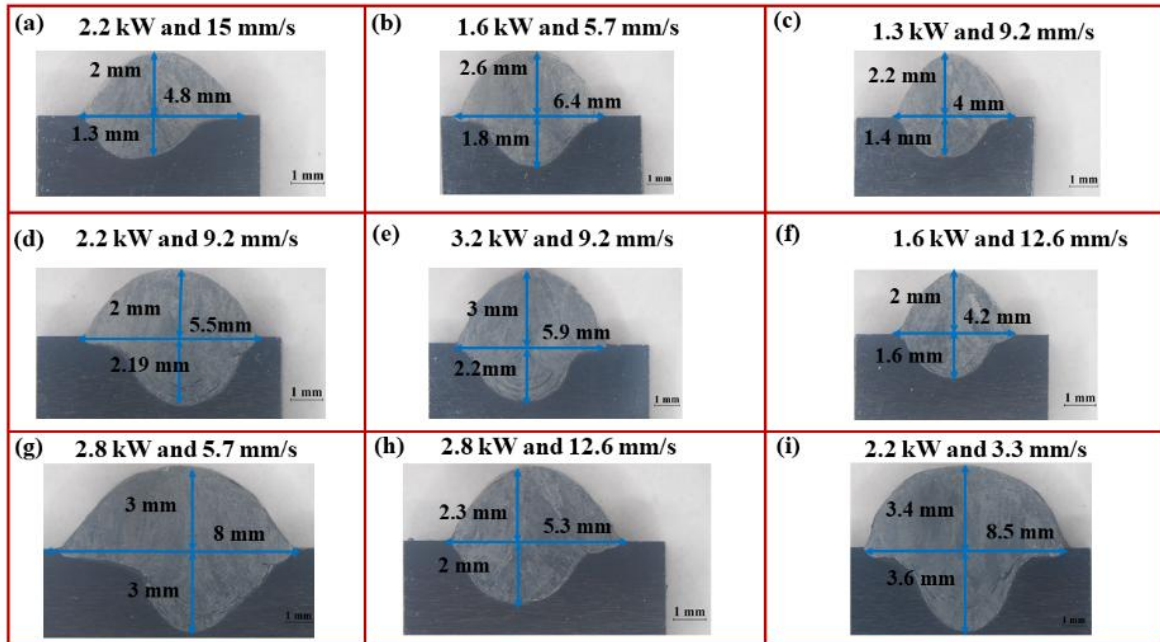


Figure 3.1: Optical macrographs of single-layer 9Cr-1Mo steel beads deposited using CMT-based WAAM under varying power and travel speed conditions. The images illustrate differences in bead geometry, surface quality, and penetration depth, enabling identification of optimal deposition attributes for full fusion and geometric stability.

3.3 Single track multi-layer deposition of 9cr-1Mo steel

The CMT based DED system, integrated with a robotic arm is employed to fabricate a thin wall structure through a layer-by-layer approach as shown in Figure 3.2a, where Figure 3.2b highlights the dimensions of the wall deposited over a stainless steel substrate, and Figure 3.2c presents the final 20-layered wall of dimensions 120 mm × 5 mm × 30 mm printed using a unidirectional scanning strategy. During the printing process, the CMT torch moves steadily along the deposition path while maintaining a constant torch-to-surface distance of 12 mm to ensure consistent arc stability and controlled metal transfer. A wide range of inter-layer dwell times, varying from 100 s to 500 s is maintained to investigate its influence on the development of residual stress within the deposited structure, and the optimized process parameters used for wall fabrication are summarized in Table 3.1. To minimize substrate movement during the deposition process and to promote mechanical stability, C-clamps are employed, which in turn contribute to the residual stress accumulation within the structure. The thermal history during deposition is captured using K-type thermocouples strategically placed at key positions to

accurately record the transient temperature distribution throughout the build cycle. Surface residual stress after the deposition of material is measured using X-ray diffraction technique (X-stress 300) utilizing $\sin^2\psi$ methodology. The probe of diameter 3 mm is used to capture the data by maintaining 10 mm over the surface. Six ψ angles having variation between -35° to 35° is adopted for the measurement. The material is selected as ferritic steel from the database to apply X-ray resilient constants and the lattice parameter d_0 . The ferritic steel properties of Young's modulus (211 GPa), Poisson's ratio (0.3), diffraction angle (156.4°), interplanar spacing (0.11708699 nm), miller indices [211], and crystal structure as cubic are considered for the evaluation residual stress. The portable XRD (X-stress 300) is utilized for measuring the surface residual stress in the longitudinal and build direction of the deposits.

Table 3.1: Optimized process parameters used in present investigation.

Parameters	Description
Current (I)	180 A
Gas flow rate	10 l/min
Shielding gas composition	80% argon and 20% CO ₂
Wire feed rate	3.2 m/min
Deposition velocity	758 mm/min
Inter-layer dwell times	100 s, 180 s, 270 s, 400 s, 450 s and 500 s

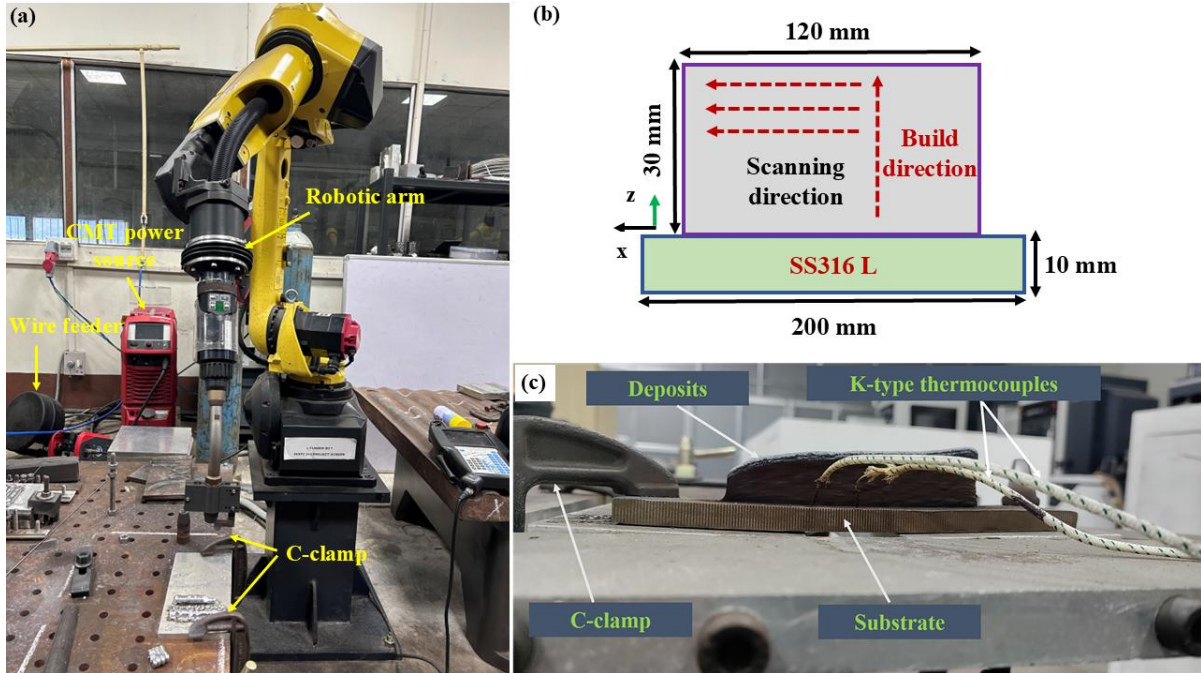


Figure 3.2: (a) Experimental setup utilized for single-track multi-layer deposition of ferritic steel; (b) scanning strategy utilized for printing thin-wall structures; and (c) fabricated 9Cr-1Mo wall.

3.4 Single track multi-layer deposition using different scan patterns

The thin wall structure of single track and multi-layered deposits of dimensions 120 mm × 5.7 mm × 50 mm are printed using CMT based DED process for varying scan patterns (Figure 3.3). On comparing the actual composition of the feedstock material and DED fabricated structures (as shown in Table 3.2), it becomes clear that the levels of the key alloying elements, chromium and molybdenum, have increased. These variations can likely be attributed to manufacturing tolerances, as welding consumables generally permit some fluctuation in their chemical composition, and the measured values fall within these acceptable limits. However, in this study, the reduction in the composition of alloying elements is mainly concentrated in the ferrite stabilizer, leading to a significantly lower chromium equivalent in the filler wire. There was also a rise in carbon content after deposition, likely due to the CO₂ in the active shielding gas. Moreover, the increased nickel and carbon content function as stabilizers for austenite in deposited material. The substrate is clamped such that the displacement boundary condition is imposed. Two different material deposition paths are adopted namely as uni-directional and bi-directional at a heat input of 310 J/mm (Figure 3.3a,

3.3b). Three different walls are fabricated at different heat input levels (232.5 J/mm, 310 J/mm, 465 J/mm) by incorporating bi-directional deposition scanning strategy (Figure 3.3e – g). Various levels of heat input are decided based on the single bead trial deposition. A continuous bead is considered stable up to 465 J/mm, beyond which, excessive material flow occurs due to high superheating of metal. For all these cases, a fixed amount of inter-layer dwell-time of 100 s is considered between the stack of layers. The mixture of argon and CO₂ gas is utilized as shielding gas for the experiment. The parameters utilized for the fabrication of thin walls are illustrated in Table 3.3.

Table 3.2: The chemical composition of ER90SB91 wire and deposited material (wt. %).

Elements	C	Cr	Mo	Mn	Ni	V	Nb	Si	O	Fe
Feed-stock material	0.07	9.1	0.9	0.4	0.4	0.21	0.05	0.25	0	Bal.
Deposited material	0.21	11.3	1.1	0.59	0.65	0.38	0.98	0.19	0.045	Bal.

Table 3.3: Deposition attributes utilized for printing a wall.

Attributes	Descriptions
Wire diameter	1.2 mm
Wire feed speed	3.2 m/min
Inter-layer dwell time	100 s
Shielding gas flow rate	10 L/min
Shielding gas composition	80% argon and 20% CO ₂
Scanning strategies	Uni-directional and Bi-directional
Heat input (Bi-directional)	465 J/mm, 310 J/mm, 232.5 J/mm

Two different material deposition paths are deployed namely as uni-directional and bi-directional at a heat input of 310 J/mm (Figure 3.3 a and b). Figure 3.3 c and d indicate that the walls printed with uni-directional scanning strategy deviate in the height along the build direction on increment of the stack of layers. The uni-directional scan leads to high peak temperature at the end of deposition and results in an abrupt change in temperature gradient along the deposition direction. More accumulation of heat energy at the end of the deposition creates an anomaly in temperature distribution. Arc starts and end points continuously alter on depositions of subsequent layers in case of bi-directional scan (Figure 3.3b). It leads to relatively uniform distribution of heat and thus regular structure can be produced. However, periodic bulges on the surface of all fabricated walls are observed that signify the stacking of layers (Figure 3.3e-g). It is inferred that the newly deposited layer on the previous one directly affects the surface quality of the printed part. The oxidation on the surface is controlled by using shielding gas. However, small quantity of oxygen is identified on the printed component (Table 2) that may lead to the formation of porosity. Variation in oxygen concentration within 9Cr-1Mo steel printed through CMT based DED process is primarily dictated by the thermal exposure duration and the oxidation kinetics intrinsic to the process. At a high heat input of 465 J/mm, the molten pool remains in the liquid phase for an extended period, facilitating enhanced interaction with the surrounding atmosphere. This prolonged exposure enables greater diffusion of oxygen into the melt, intensifying surface oxidation reactions and leading to increased oxygen entrapment in the solidifying metal. In contrast, when a lower heat input of 232.5 J/mm is employed, the molten pool undergoes rapid solidification, significantly shortening the time available for gas-metal interaction. This limits the extent of oxidation and thus results in reduced oxygen pickup. The intermediate heat input setting of 310 J/mm offers a transitional regime, where moderate thermal exposure allows for a balanced level of oxygen absorption. This observed trend corresponds well with foundational principles in welding science, where oxygen incorporation in weld metal is strongly influenced by the thermal profile of the process. As described by Eagar et al. [147], the degree of oxygen contamination in arc welding operations is closely tied to heat input, which governs both the longevity and reactivity of the molten phase when exposed to ambient conditions. All these issues are addressed from the perspective of temperature distribution, solidification behavior, microstructural analysis and finally mechanical properties.

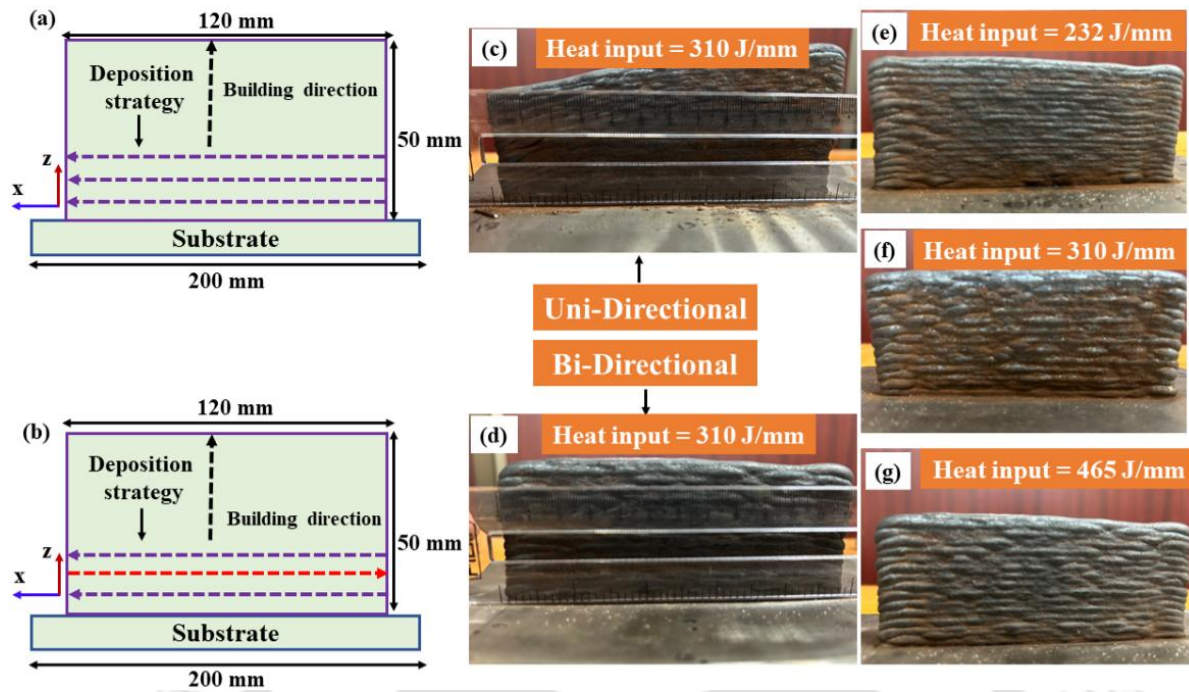


Figure 3.3: (a, b) Printing strategy for fabricating wall; (c, d) Scanning strategy at heat input 310 J/mm; (e – g) Deposited pattern for bi-directional scan at different heat inputs.

The deposited walls are cut from three different locations (top, middle, and bottom) using wire electric discharge machining (EDM) process. The samples are etched using Villella's reagent (100 ml ethanol + 5 ml hydrochloric acid + 1 g picric acid). The microstructure is evaluated by Carl Zeiss SEM instrument equipped with an Oxford energy dispersive spectroscopy (EDS) detector. A few selected specimens were subjected to electron backscattered diffraction (EBSD) analysis using FEG-SEM (Model FEI Nova Nano), which operated at 20 kV and was equipped with a TSL-OIM acquisition system. EBSD samples are prepared by electro polishing in a solution containing 90% ethanol and 10% perchloric acid at 30 V and -30°C . EBSD scans for all the samples are performed at 20 kV with step size of $0.1\text{ }\mu\text{m}$. Post-processing of the microstructure is performed to obtain image quality (IQ), inverse pole figure (IPF) map, and phase evolution map. XRD analysis of the as-cast specimen was performed using the Rigaku Ultima IV X-ray diffraction system with $\text{Cu-K}\alpha$ (0.154 nm) radiation. Specimens were scanned from 20° to 90° with a scan speed of $1^{\circ}/\text{min}$. The presence of different phases within the samples are identified using XRD test. The portable XRD (X-

stress 300) is utilized for measuring the surface residual stress in the longitudinal and build direction of the deposits. A few selected specimens were prepared and analyzed under the transmission electron microscope (TEM-Model: JEOL 2200 FS attached with Oxford EDS detector). Thin sheets were cut using an EDM wire cutter and thinned down to 50 μm . Vickers microhardness test (Omni-Tech-S. No.–551, Model F. AUTO) is performed by applying a load of 300 g on polished samples with a dwell time of 10 s. Tensile tests are performed on median 250 kN testing machine (BISS Model: MEDIAN 250) with a cross speed of 1 mm/min at room temperature. Tensile samples are extracted along the deposition directions following the ASTM standard E8. While testing, an extensometer of gauge length 25 mm is utilized. Fracture morphologies of different samples are observed by SEM.

3.5 Multi-track-multi-layered deposition of 9Cr-1Mo steel

For the fabrication of rectangular 9Cr–1Mo steel components, an optimized set of process parameters is employed to ensure dimensional accuracy and structural integrity (Table 3.4). The deposition is carried out in a multi-track, multi-layer configuration, and the scanning strategies are systematically varied to examine their influence on thermal behavior and stress evolution. As illustrated in Figure 3.4, six distinct path designs are implemented, classified according to the orientation of the deposition trajectories with respect to the substrate length. Deposition tracks aligned parallel to the longer edge (80 mm) are referred to as longitudinal, while those perpendicular to it are termed transverse (Figure 3.4 a and b). In the spiral-in strategy, deposition begins at the outer boundary and advances inward in a helical fashion, whereas the spiral-out pattern starts at the center and expands outward (Figure 3.4 c and d). The inclined pattern follows a diagonal raster path oriented at approximately 45° to the length. The circular strategy involves concentric paths progressing radially from the center to the periphery (Figure 3.4e). These programmed scanning trajectories, followed by the arc during deposition, form the basis for assessing the role of path geometry in controlling thermal distribution, layer buildup, and subsequent material response. A uniform hatch spacing of 3.53 mm is employed for all scan patterns in conjunction with a constant heat input of 222.2 J/mm. This spacing corresponds to two-thirds of the bead width, ensuring optimal track overlap and consistent layer deposition, as suggested by Suryakumar et al. [34]. Accordingly,

a multi-track, multi-layer stack with dimensions of $1.6 \text{ mm} \times 50 \text{ mm} \times 80 \text{ mm}$ are deposited to fabricate the rectangular part.

Table 3.4: Deposition attributes utilized for printing rectangular components.

Attributes	Descriptions
Power	2.8 kW
Shielding gas composition	80% Argon and 20% CO ₂
Gas flow rate	10 L/min
Wire feed rate	3.2 m/min
Inter-layer dwell times	1100 s
Deposition velocity	758 mm/min
Scanning strategy	Longitudinal, transverse, spiral-in, spiral-out, inclined and circular

Samples for metallurgical analysis are extracted from the central region along the build direction at the mid-length of the rectangular deposits to ensure representative assessment of the microstructure. Precision sectioning is performed using wire EDM to minimize thermal damage and preserve microstructural integrity. In order to develop thermo-metallurgical-mechanical models in accordance with Pohjonen's theory [148], solid-state phase transformation (SSPT) behavior is characterized through dilatometric experiments. Standard cylindrical samples with dimensions of $80 \text{ mm} \times \text{Ø } 6 \text{ mm}$ are extracted from the printed components fabricated using each scanning strategy. The tests are carried out using a Gleeble 3800 thermomechanical simulator, where each specimen is subjected to a controlled thermal cycle comprising linear heating at 100°C/s to a peak temperature of 1100°C , followed by a 10 s isothermal hold, and cooling at 0.1°C/s . Transformation-induced strains are continuously recorded throughout the thermal cycle, providing essential input data for modeling phase

evolution and stress development under realistic thermal conditions. Residual stress present in printed rectangular parts are evaluated using portable XRD based on the $\sin^2\psi$ method.

3.6 Summary

The systematic deposition studies on 9Cr–1Mo steel using a CMT-based DED system are carried out in a stepwise manner, beginning with single-track beads and progressing to multi-track, multi-layer walls, to establish the correlation between process conditions, bead geometry, and residual stress evolution. In the single-layer stage, bead dimensions such as penetration depth, height, and width are evaluated to confirm complete substrate fusion and geometric stability, revealing that higher power with lower travel speed increased penetration but risked excessive bead spreading, while intermediate settings produced balanced geometries more suitable for multi-layer stacking. Thin-wall structures fabricated with a unidirectional scanning approach further enabled the investigation of inter-layer dwell time, where thermocouple-based temperature monitoring and XRD residual stress measurements demonstrated that dwell strongly influenced thermal accumulation and stress distribution across the wall height. Extending to multi-layer walls, both uni-directional and bi-directional strategies are applied at varying heat inputs, showing that deposition remained stable up to 465 J/mm and that bi-directional paths provided superior thermal balance and reduced stress localization compared to uni-directional passes. The study is finally expanded to rectangular multi-track, multi-layer components, where six distinct scanning trajectories such as longitudinal, transverse, spiral-in, spiral-out, inclined, and circular are implemented to alter heat flow orientation relative to the substrate. With a fixed hatch spacing of two-thirds bead width and constant heat input, these patterns are shown to critically affect thermal distribution, layer uniformity, and the resulting material responses. Moreover, dilatometric studies are conducted to reveal the phase transformation kinetics of printed 9Cr-1Mo components. Collectively, the investigation establishes that process optimization involving heat input, dwell time, and scan geometry is fundamental for tailoring bead morphology, mitigating residual stresses, and achieving high-quality 9Cr–1Mo steel components through CMT wire-based DED system.



Computational work

4.1 General background

In-situ monitoring of additive layer characteristics during wire-based DED process remains a major challenge because of the extreme thermal gradients, rapid solidification rates, and restricted accessibility of the melt pool. As a result, direct experimental tracking of temperature fields, residual stress evolution, and phase transformations is often impractical. At the same time, optimizing process parameters through conventional trial-and-error experiments is not only time-consuming but also increases the overall cost of product development. These limitations have established computational modeling as a powerful and necessary tool for process analysis and optimization in additive manufacturing. Numerical simulations, particularly FE based approaches, are widely employed to investigate the coupled thermo-mechanical phenomena occurring during DED. Such models solve complex governing equations under realistic boundary conditions, thereby enabling detailed predictions of thermal histories, phase evolution, residual stresses, and distortion. However, despite their accuracy, high-fidelity FE simulations are computationally expensive, require significant expertise to set up, and depend heavily on commercial software platforms that are not freely available. This creates barriers to their extensive use in industrial and research applications. To overcome these constraints, hybrid approaches that integrate numerical simulations with machine learning (ML) have gained prominence. In the present study, FE-based thermal and mechanical models were first developed and calibrated against experimental measurements to ensure physical reliability. Once validated, extended simulations were conducted to generate large, high-quality datasets representing the physics of deposition. These datasets were then used to

train ML algorithms, where hyperparameter tuning was performed to achieve optimal model performance. The trained models, achieving higher accuracy, are subsequently deployed for rapid predictions and validated against independent experimental and simulation results. By combining the rigorous physical basis of numerical modeling with the efficiency of data-driven learning, this integrated framework significantly reduces computational cost while retaining predictive fidelity. Such hybrid computational strategies represent a transformative approach for advancing DED, enabling accelerated process optimization and enhancing the scientific understanding of complex additive manufacturing phenomena.

4.2 Numerical model for simulating single track deposits

A 3D thermal model is developed following the FE method where a double-ellipsoidal heat source model is implemented [149]. The heat source model parameters are calibrated from single-bead experiment (Table 1). The elemental birth and death technique is utilized for material deposition following a scanning path activated by the user-defined Python program [150]. The numerically calculated deposited track is parabolic in nature. It is obtained by creating a geometry of the same dimension as observed from CMT deposits. In the part module, the deactivating and activating of the element is performed using a model change option present in the interaction module. The substrate and deposited material are set to ambient condition (25°C) as initial condition. During the deposition of the material, heat loss from the deposited component consists of radiation and convection mode of heat transfer. A convective heat transfer coefficient of $800 \text{ Wm}^{-2}\text{C}^{-1}$ is considered for the bottom surface of the substrate and $25 \text{ Wm}^{-2}\text{C}^{-1}$ for the remaining part. In the radiative mode of heat transfer, the emissivity of a “grey” body is considered as 0.8. The transient heat transfer conduction in a moving reference frame is expressed as

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + \dot{Q} = \rho C_p \left(\frac{\partial T}{\partial t} - v \frac{\partial T}{\partial x} \right) \quad (3.1)$$

where k is the thermal conductivity, ρ is density, C_p is specific heat and $\dot{Q}$ is the volumetric heat source. The term $-v\rho C_p \left(\frac{\partial T}{\partial x} \right)$ depicts the coordinate transformation for the movement of

the heat source along the deposition length. The boundary conditions that are utilized to solve the above differential equations (1) are prescribed as follows:

Dirichlet or Essential boundary condition: It represents that the initial temperature of the model is at ambient temperature (T_0) i.e at time $t = 0$

$$T(x, y, z, t = 0); T_0 = 25^\circ\text{C} \quad (3.2)$$

Natural or Neumann boundary condition: Heat transfer from the deposited sample and substrate:

$$-\left\langle \frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}, \frac{\partial T}{\partial z} \right\rangle \hat{n} = \varepsilon \sigma (T^4 - T_0^4) + h (T - T_0) \quad (3.3)$$

where $\hat{n}$, σ , ε , and h represent the unit normal surface vector, Stefan-Boltzmann constant ($5.6704 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$), ε is the emissivity of a “grey” body (0.4) and h is the convective heat transfer coefficient. The asymmetric power density distribution is implemented through the double-ellipsoidal heat source model [103]. The fusion zone generally displays a teardrop shape because the heat source's motion and the flow of liquid metal within the molten pool are compensated by adjusting thermal conductivity in the conduction frame of the heat transfer model. The mathematical expression for this volumetric heat source in the front and rear part of the arc is represented by

$$q_f(x, y, z) = \frac{6\sqrt{3}(f_f \eta P)}{\pi \sqrt{\pi a_f b c}} \exp \left[-3 \left(\frac{x^2}{a_f^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \right) \right]; \text{ if } x \geq vt \quad (3.4)$$

$$q_r(x, y, z) = \frac{6\sqrt{3}(f_r \eta P)}{\pi \sqrt{\pi a_r b c}} \exp \left[-3 \left(\frac{x^2}{a_r^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \right) \right]; \text{ if } x < vt \quad (3.5)$$

$$\text{where } f_f = \frac{2a_f}{a_f + a_r}; \quad f_r = \frac{2a_r}{a_f + a_r}; \quad f_f + f_r = 2;$$

$$\dot{Q} = q_f + q_r \quad (3.6)$$

Here, a_f and a_r are the length of the front and rear parts of the double ellipsoidal heat source, b is the width, and c is the depth of the heat source. P represents the power of arc, and η is the thermal efficiency. f_f and f_r are the factors for distributing the power source to the front and

rear of the heat source. q_f and q_r are the distribution of power in the front and rear quadrants of the heat source utilized. The number of steps required for the deposition along the length is decided by the velocity (v) and is expressed as [42]

$$N = \frac{L}{v\Delta t} \quad (3.7)$$

A set of numerical simulations are performed to obtain the transient temperature profile and peak temperature during deposition. This simulation consists of depositing a single layer on a substrate of dimension $120 \times 90 \times 10 \text{ mm}^3$ as shown in Figure 4.1. The temperature dependent thermo-physical properties of P91 (wire) and 316L (substrate) are utilized for the numerical model [151,152]. These properties are depicted in Figure 4.2 and Table 4.2. A fine mesh is associated with the deposited part. The activation of the element is performed as per the deposition rate. The mesh size with shape function (linear and quadratic) is optimized with respect to the peak temperature of the system. The maximum temperature obtained for linear and quadratic type of elements for each mesh is depicted in Figure 4.3. There is not much difference in the peak temperature of linear and quadratic elements, however, the simulation time with quadratic mesh is much more. Therefore, the linear mesh is considered in the present work with total number of 108000 elements. A set of numerical simulations are performed to obtain the transient temperature profile and peak temperature during deposition. It has been realized that the significant impact on the variation of temperature are power and velocity [25]. For each deposition attribute, eleven different levels are considered where the dataset is depicted in Table 4.3. A total 121 cases of numerical simulations are performed and accordingly the results are modified.

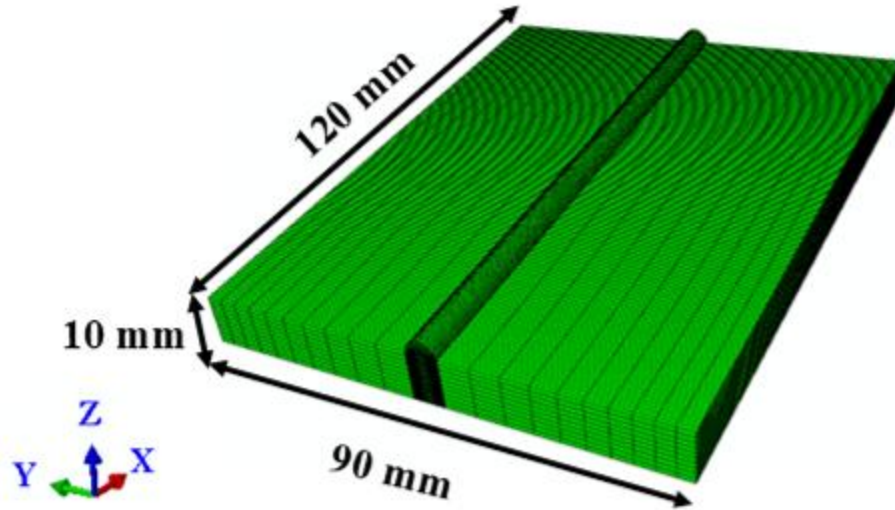


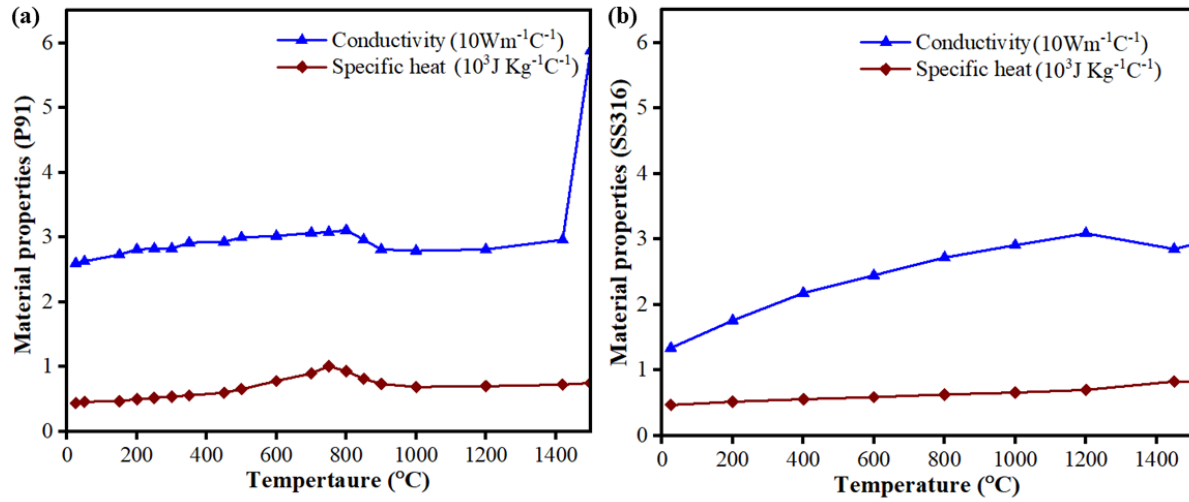
Figure 4.1: Illustration of the numerical models for simulating single track deposition of 9Cr-1Mo steel.

Table 4.1: Heat source parameters utilized for numerical simulation

Parameter	Value
<i>Width (mm)</i>	2.7
<i>Layer thickness (mm)</i>	2
f_f	0.56
f_r	1.44
a_f (mm)	2.5
a_r (mm)	6.5
b (mm)	$width = 2.7$
c (mm)	$depth = 1.5$
<i>Thermal efficiency (η)</i>	0.85

Table 4.2: Thermo-physical properties of 9cr-1Mo and SS316

Material	Latent heat of fusion (J/kg)	Density (kg/m ³)	Solidus temperature (°C)	Liquidus temperature (°C)
P91	260×10^3	7770	1420	1500
SS316	272×10^3	7800	1385	1450

**Figure 4.2:** Thermal conductivity and specific heat capacity of (a) P91 and (b) SS316 material [16, 17].

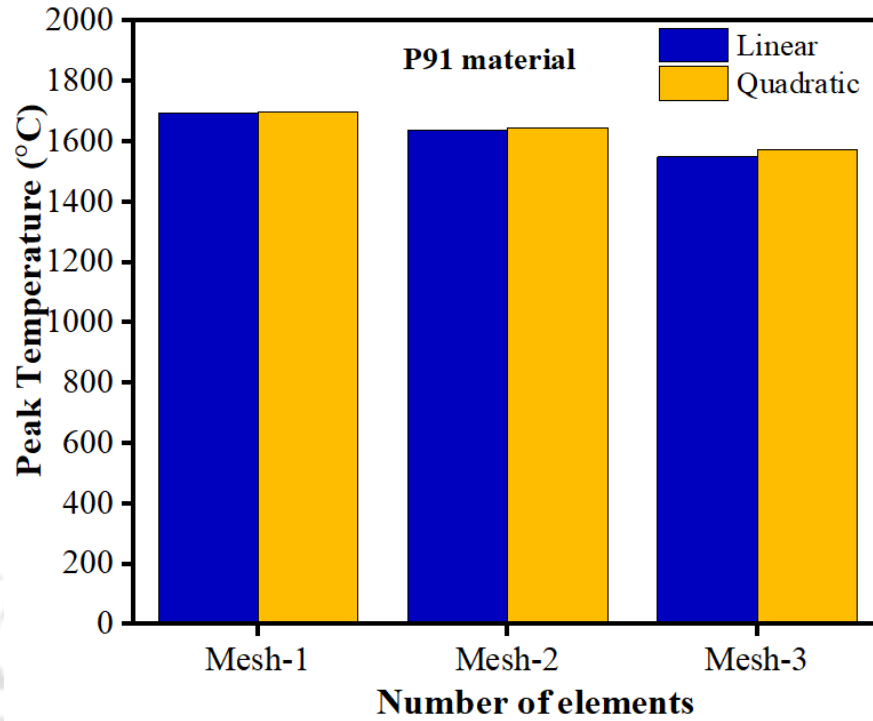


Figure 4.3: Comparison of the peak temperature for different mesh size and elements for 9Cr-1Mo deposits.

Table 4.3: Attributes utilized for generating transient temperature dataset using numerical simulation for single track deposition.

Power (W)	Velocity (mm/s)										
	3.3	4.5	5.6	6.8	7.9	9.1	10.3	11.5	12.6	13.8	15
1280	S ₁	S ₂	S ₃	S ₄	S ₅	S ₆	S ₇	S ₈	S ₉	S ₁₀	S ₁₁
1468	S ₁₂	S ₁₃	S ₁₄	S ₁₅	S ₁₆	S ₁₇	S ₁₈	S ₁₉	S ₂₀	S ₂₁	S ₂₂
1656	S ₂₃	S ₂₄	S ₂₅	S ₂₆	S ₂₇	S ₂₈	S ₂₉	S ₃₀	S ₃₁	S ₃₂	S ₃₃
1844	S ₃₄	S ₃₅	S ₃₆	S ₃₇	S ₃₈	S ₃₉	S ₄₀	S ₄₁	S ₄₂	S ₄₃	S ₄₄
2032	S ₄₅	S ₄₆	S ₄₇	S ₄₈	S ₄₉	S ₅₀	S ₅₁	S ₅₂	S ₅₃	S ₅₄	S ₅₅
2220	S ₅₆	S ₅₇	S ₅₈	S ₅₉	S ₆₀	S ₆₁	S ₆₂	S ₆₃	S ₆₄	S ₆₅	S ₆₆
2408	S ₆₇	S ₆₈	S ₆₉	S ₇₀	S ₇₁	S ₇₂	S ₇₃	S ₇₄	S ₇₅	S ₇₆	S ₇₇

2596	S ₇₈	S ₇₉	S ₈₀	S ₈₁	S ₈₂	S ₈₃	S ₈₄	S ₈₅	S ₈₆	S ₈₇	S ₈₈
2784	S ₈₉	S ₉₀	S ₉₁	S ₉₂	S ₉₃	S ₉₄	S ₉₅	S ₉₆	S ₉₇	S ₉₈	S ₉₉
2972	S ₁₀₀	S ₁₀₁	S ₁₀₂	S ₁₀₃	S ₁₀₄	S ₁₀₅	S ₁₀₆	S ₁₀₇	S ₁₀₈	S ₁₀₉	S ₁₁₀
3160	S ₁₁₁	S ₁₁₂	S ₁₁₃	S ₁₁₄	S ₁₁₅	S ₁₁₆	S ₁₁₇	S ₁₁₈	S ₁₁₉	S ₁₂₀	S ₁₂₁

The structural model is formulated to determine the displacement of the printed track. This non-linear mechanical analysis can be considered as a quasi-static incremental analysis based on a Lagrangian frame of reference and is expressed as [153]

$$\nabla \sigma + B = 0 \quad (3.8)$$

where σ represents second order Cauchy stress tensor and b is the sum of the body force vector. The thermo-elastoplastic model considers material deformation in the plastic zone and elastic recovery. The stress and strain from the Hooke's law of elasticity are expressed as [154]

$$\sigma = C \varepsilon^e \quad (3.9)$$

where C is the stiffness matrix of fourth-order and ε^e is the second-order elastic tensor. The total incremental strain ($\Delta \varepsilon$) induced is the combination of thermal strain ($\Delta \varepsilon^{th}$), elastic strain ($\Delta \varepsilon^e$), plastic strain ($\Delta \varepsilon^p$), and strain developed due to solid-state phase transformation ($\Delta \varepsilon_{ij}^v$) is expressed as [155].

$$\Delta \varepsilon_{ij}^{total} = \Delta \varepsilon_{ij}^e + \Delta \varepsilon_{ij}^{th} + \Delta \varepsilon_{ij}^p + \Delta \varepsilon_{ij}^v \quad (3.10)$$

The increment of stress developed from the elastic strain is given by [138]

$$\Delta \sigma_{ij}^E = D_{ijlm} \Delta \varepsilon_{lm}^E \quad (3.11)$$

where D_{ijlm} is the elastic stiffness matrix evaluated from the modulus of elasticity (E) and

Poisson's ratio μ as given by

$$D_{ijlm} = \frac{E}{1+\mu} \left[\frac{1}{2} (\delta_{il}\delta_{jm} + \delta_{lm}\delta_{ij}) + \frac{\mu}{1-2\mu} \delta_{ij}\delta_{lm} \right] \quad (3.12)$$

where $\delta_{ij}, \delta_{il}, \delta_{jm}, \delta_{lm}$ are Kronecker delta whose value is unity for $i = j$ else, it's zero for $i \neq j$. The Von Mises yield criteria is used for plastic deformation. The thermal strain is expressed as

$$\Delta \varepsilon_{lm}^{th} = \alpha \delta_{lm} \Delta T \quad (3.13)$$

where α is the coefficient of thermal expansion and ΔT is a transient temperature increment.

By applying the suitable boundary conditions, stress, strain, and displacement at nodal points are evaluated by applying the Newton-Raphson iteration scheme. The effective stress known as Von Mises stress is computed to decide whether the state of stress is within the elastic limit or not. However, the yield strengths of the metallic material decrease on increasing the temperature. Hence, suitable temperature-dependent yielding criteria and flow rules are applied. The isotropic hardening behavior is followed in the present model.

4.3 Numerical model for simulating single track multi-layer deposits

The numerical model of the DED process triggers thermo-mechanical data generation. The continuous re-melting of a deposited layer leads to an approximately flat bead profile after a certain number of layers. Therefore, the surface profile is considered rectangular with similar molten pool dimensions without violating the energy conservation. The symmetric solution domain as well as thermal boundary conditions are depicted in Figure 4.4d. The contact resistance at the bottom surface (convective mode) is introduced by using a high value of heat transfer coefficient of $800 \text{ Wm}^{-2}\text{C}^{-1}$ in comparison to $25 \text{ Wm}^{-2}\text{C}^{-1}$ for the rest of the part. The transient heat conduction equation in a moving reference frame along with boundary conditions is solved to obtain the temperature field [44]. Clamps and encasters impose the mechanical boundary conditions. The solidus and liquidus temperature of 1420°C and 1500°C for ferritic steel, 1385°C and 1450°C for austenitic steel is considered. The temperature-

dependent thermal and mechanical properties for both the deposited (P91) and base material (SS 316) are considered from independent literature [156,157]. The arc heat is represented through the double-ellipsoidal heat source model. The thermal history is implemented as a predefined load for structural analysis for the same solution domain. The inertia by the molten droplet has a negligible impact on the DED process. Hence, mechanical analysis is performed as a quasi-static nature with the Lagrangian reference frame. Material behavior is considered elastic recovery and induced plasticity following isotropic hardening rule in an incremental way. Elastic behavior follows generalized Hooke's law with temperature-dependent Poisson's ratio and modulus of elasticity. The von Mises yield criteria and Prandtl Reuss flow rule are implemented in the present analysis. Temperature-dependent plastic strains at a strain rate of 0.003s^{-1} are considered from independent literature for P91 material [158].

The deposition of molten droplets within the solution domain is accounted by element birth and death technique. The required geometry of the component including the substrate material is formed first and meshing is performed for the whole domain. The volume of the thin wall is deactivated first and the elements confined to the bead is activated. In this case, the volume flow rate of feeding material is equivalent to volume per unit time along the welding torch direction. The bead width and height (layer thickness) are kept fixed, and the equivalent volume of bead is adjusted along the torch velocity vector. It is assumed that the current activated elements are excluded from any thermal load in the current step and the thermo-physical properties are implemented in this step. Figure 4.4(e) demonstrates the progressive steps of activation of elements in the DED process. Inter-layer dwell times are implemented using user subroutines for each printed layer. All the simulations are performed on a Desktop PC having a configuration of Intel(R) core (TM) i5-6500 CPU with 32 GB RAM. The simulation time is noted down from the "DAT file" on completion of each job at a specific dwell time.

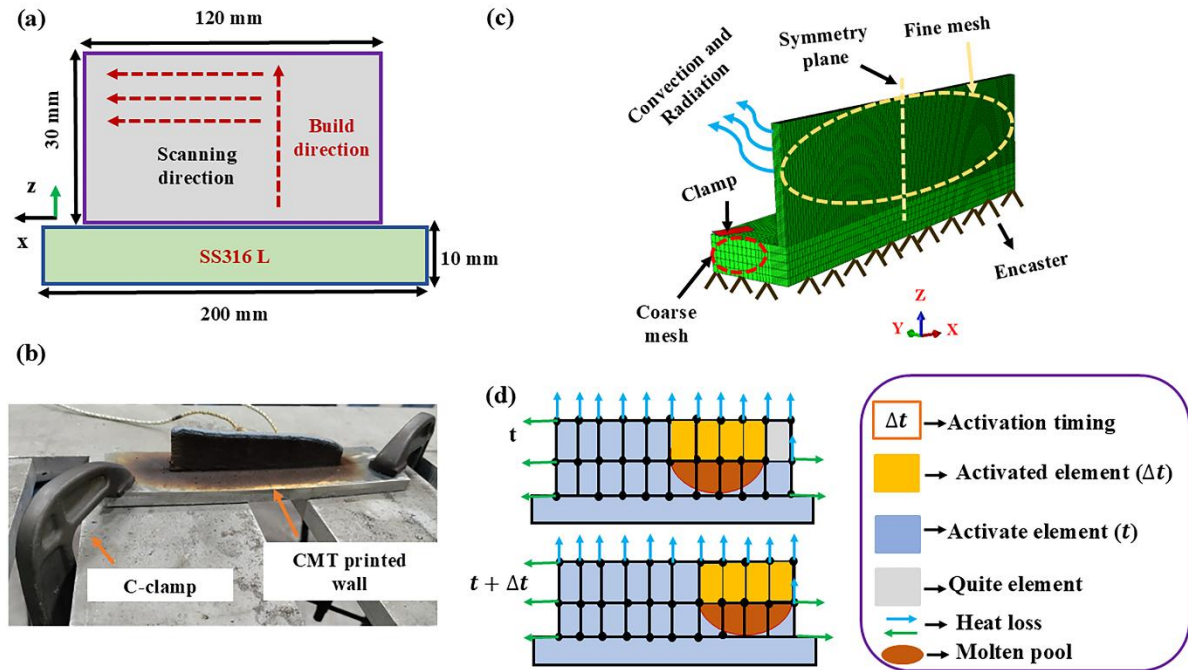


Figure 4.4: (a) Schematic illustration of the scanning strategy and dimensions of printed wall; (c) Printed wall by CMT process; (d) Computational domain with boundary conditions; and (e) Interpretation of the sequential activation and deactivation of the element.

Thermo-mechanical model depicts the variation of temperature field and residual stress evolution in single-track deposition of ferritic steel. Initially, a transient thermal profile during the deposition of material was accomplished through heat transfer analysis. Secondly, the thermal load is utilized for computing residual stress profile from structural analysis. A flow chart consisting of steps involved in thermo-mechanical analysis is shown in Figure 4.4. The effect of solid-state phase transformation and transformation-induced plasticity is neglected in the present analysis as it has an insignificant effect on residual stress generation.

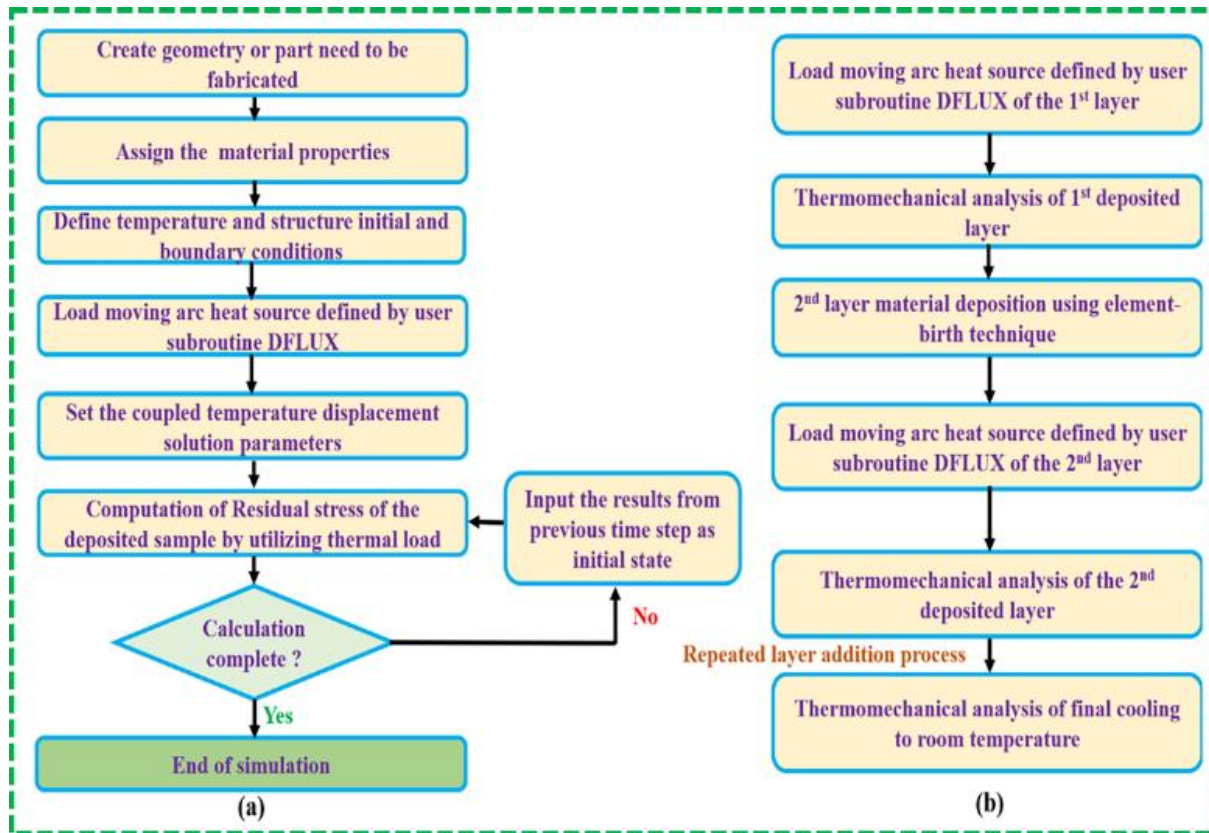


Figure 4.5: Illustration of the sequential steps followed for the development of thermo-mechanical model.

4.4 Numerical model for simulating multi-layer deposits on incorporating scan pattern

A FE based thermo-mechanical model is developed to replicate the CMT-based DED process. The model incorporates gradient meshing and element activation along the tool path to ensure accurate resolution of thermal and mechanical gradients. The thermal and mechanical boundary conditions are depicted in Figure 4.6. The density of solid and liquid phases of 9Cr-1Mo steel is assumed to be constant, and the latent heat of fusion or solidification is incorporated into the heat transfer model. Temperature-dependent thermo-physical properties of 9Cr-1Mo steel is implemented in the model [159]. The material behavior is modeled as isotropic to simplify the analysis. The temperature field obtained from the thermal model is applied as a thermal load for stress analysis, following a sequentially coupled thermo-mechanical analysis. A CAD model of the thin wall, designed according to the dimensions of the printed wall is depicted in Figure 4.6a. Only half of the symmetric geometry is considered to reduce computational time. A double-ellipsoidal heat source model [160] is used to represent

arc energy. The heat loss due to convection and radiation is accounted at the boundaries (Figure 4.6 b). The heat transfer model is rigorously calibrated by adjusting heat transfer coefficients to comply with experimental conditions (Figure 4.6c). The solution geometry consists of fine and coarse meshes, comprising 108,000 elements (Figure 4.6b). DC3D8R and C3D8R elements are utilized for thermal and mechanical analysis, respectively. The deposition process is simulated using an element birth and death technique via user-defined subroutines. Initially, all elements assigned to the fabricated structure are deactivated and then sequentially activated along the tool path. A cooling period of 100 seconds between stack of layers is implemented using the DFLUX subroutine. In order to simulate the different scan path namely uni-directional and bi-directional, material depositions are modified through python scripts and movement of heat source are incorporated in DFLUX subroutines on modifying the coordinates of start and end point. The stress analysis is performed on Lagrangian reference frame. Under static equilibrium conditions, thermo-elastic-plastic material model is considered. The elastic stress follows generalized Hooke's law, whereas von Mises yield criteria with Prandtl Reuses flow rule and isotropic hardening behavior is considered for plastic flow of material. Temperature dependent modulus of elasticity, Poisson's ratio and yield strength at strain rate of 0.03 s^{-1} is incorporated from independent literature [158]. The encastre mechanical constraint in negative Z-direction and clamping conditions are applied to enforce actual boundary conditions.

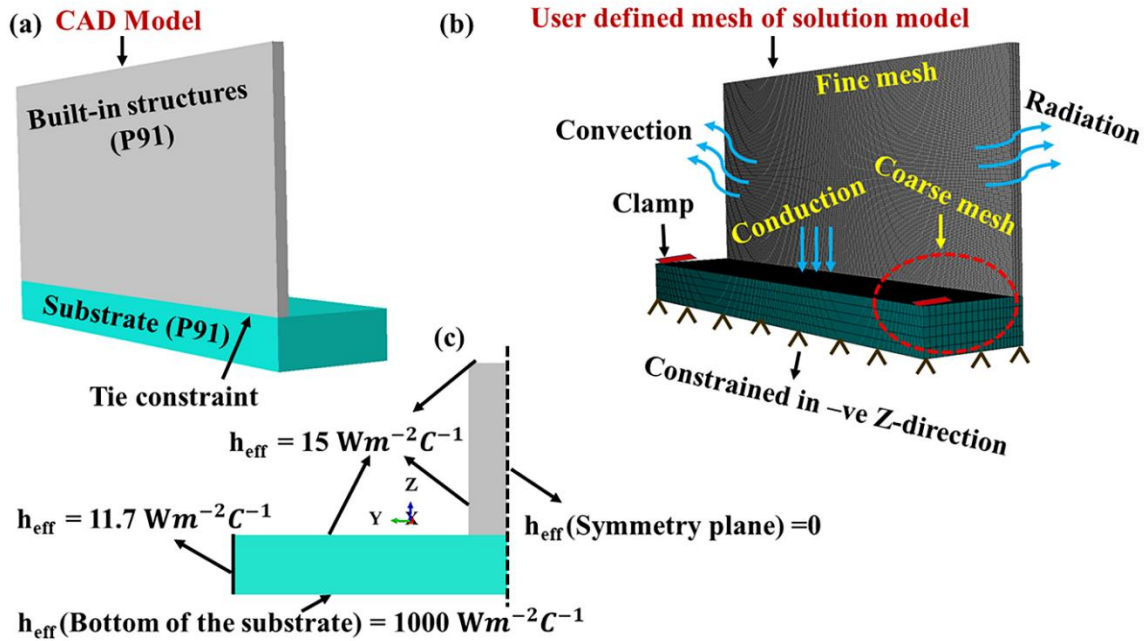


Figure 4.6: (a) Schematic representation of the computer-aided design (CAD) model for the printed thin-wall structure used in the directed energy deposition (DED) process, showing the intended geometry. (b) Solution geometry with applied thermal and mechanical boundary conditions, including heat input and fixed constraints for finite element analysis. (c) Effective heat transfer coefficients are defined on different surfaces to account for convective heat losses during the deposition process.

4.5 Thermal-metallurgical-mechanical (TMM) model

A FE based thermal-metallurgical-mechanical (TMM) model is established to simulate the CMT based DED process. The model features gradient meshing and sequential element activation along the tool path to accurately capture localized thermal and mechanical behavior. A mesh sensitivity study is conducted to optimize the distribution element in both the deposited material and the substrate, ensuring a balance between computational efficiency and solution accuracy. Heat transfer model is meticulously calibrated by tuning the heat transfer coefficients to reflect the experimental boundary conditions accurately. The simulation domain incorporates a multi-resolution meshing strategy, comprising a total of 16,244 linear hexahedral elements. TMM model coupling is achieved by employing DC3D8R elements for thermal analysis and C3D8R elements for mechanical analysis. The deposited geometry is catered with sequential element activation in accordance with the predefined tool path through

user-defined subroutines. The interlayer cooling time of 1100 s is defined between successive layers.

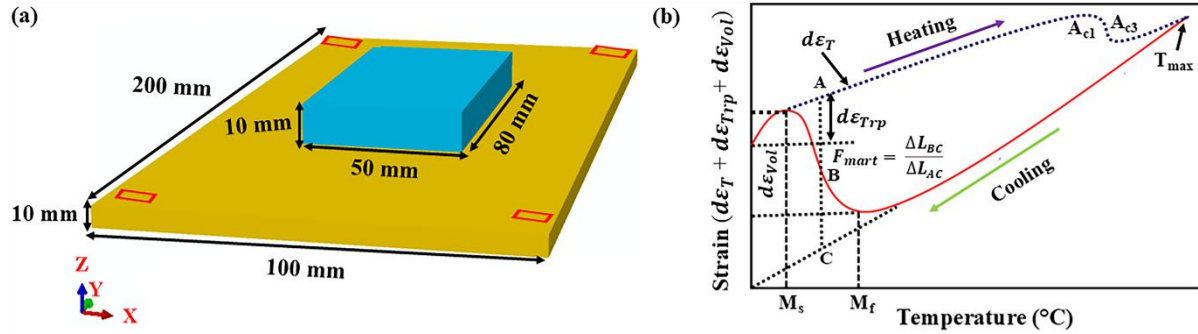


Figure 4.7: (a) CAD model of the rectangular component designed for DED process; and (b) significant elements of dilatometric strain during heating and cooling cycles.

The thermal and mechanical boundary conditions are outlined in Figure 4.7a. A double ellipsoidal heat source model is employed to represent the arc heat input including the energy contained in deposited bead. Density of 9Cr-1Mo steel is treated as constant across solid and liquid phases, while latent heat associated with phase change is incorporated into the thermal model. Temperature-dependent other thermo-physical properties are defined in this TMM model [156,161,162]. The convective flow of liquid metal within the molten metal is approximated by enhancing the thermal conductivity by a factor of five near the liquidus temperature, ensuring turbulent effect of heat transport in the liquid phase [163]. The material behavior is assumed as isotropic to simplify the analysis. The thermal history and phase transformation results from the thermo-metallurgical simulation are subsequently applied as inputs for the mechanical stress analysis, using a sequentially coupled approach.

The initial microstructure of 9Cr-1Mo steel is tempered martensite. During heating, tempered martensite can revert to austenite, and at sufficiently high local temperatures, the austenite may partially transform into δ -ferrite. However, the most influential transformations are martensite-to-austenite ($M \rightarrow A$) during heating and the reverse austenite-to-martensite ($A \rightarrow M$) during cooling. These transformations are accompanied by volumetric changes and influence directly in stress evolution. In a layer-by-layer deposition process, martensite formed in earlier passes is repeatedly exposed to reheating by subsequent layers. This reheating can cause partial tempering of martensite. However, the tempering kinetics of 9Cr-1Mo steel are

relatively sluggish since a holding time of ~ 2 h at 732°C is required to achieve significant tempering, which far exceeds the short dwell times of layers [164]. Therefore, the tempering induced during deposition is assumed negligible and the microstructural evolution in 9Cr-1Mo steel during arc-based DED is approximated as

$$F_A + F_M = 1 \quad (3.14)$$

where F_A and F_M are the volume fractions of austenite and martensite, respectively. This indicates that the austenite and martensite evolve dynamically during deposition. Figure 4.8 depicts two schematic illustrations of thermal histories relevant to arc-based DED: a single-pass deposition and a multi-pass deposition. In the single-pass case, the thermal profile exhibits a single sharp peak above the austenitization temperature (A_{C3}), followed by cooling to below the martensite finish temperature (M_f). Under this condition, 9Cr-1Mo steel undergoes a complete $M \rightarrow A$ transformation during heating and a full $A \rightarrow M$ transformation during cooling. The kinetics of these transformations are typically captured through phenomenological models. In this study, the $M \rightarrow A$ transformation during heating is approximated as a linear function of temperature

$$F_A = \frac{T - A_{C1}}{A_{C3} - A_{C1}} \quad (3.15)$$

where A_{C1} and A_{C3} denote the austenite start and finish temperatures for 9Cr-1Mo steel, respectively. The reverse transformation from austenite to martensite during cooling is described using the Koistinen–Marburger (K–M) equation, which relates the fraction of martensite as

$$F_{mart}(T) = 1 - \exp[-k(M_{start} - T)] \quad (3.16)$$

$$M_{final} \leq T \leq M_{start}$$

where F_{mart} is the volume fraction of martensite at a given temperature T , M_{start} and M_{final} are the martensite start and finish temperatures, and k is the transformation rate constant, which

governs the sharpness of the transformation. To determine the material-specific constant k , experimental dilatometry data is utilized. The dilatation $\Delta L(T)$, measured as a function of temperature, is normalized to represent the martensite fraction using the relation [26]

$$F_{mart}(T) = \frac{\Delta L - \Delta L_{min}}{\Delta L_{max} - \Delta L_{min}} \quad (3.17)$$

where ΔL_{min} and ΔL_{max} are the minimum and maximum dilatation values observed over the transformation interval, respectively. The normalized dilatation values effectively represent the progression of martensitic transformation. By rearranging the KM equation (Eq. 3.16 and 3.17), the constant k can be computed from the experimental data as

$$k = -\frac{\ln(1 - F_{mart})}{(M_{start} - T)} \quad (3.18)$$

Above expression allows the direct evaluation of k using known values of T , F_{mart} and M_{start} . In this study, the value of k is calculated for each valid data point within the transformation range. To ensure accuracy and minimize numerical artefacts, only intermediate transformation states are considered specifically those where the martensite fraction lies within a stable, central portion of the transformation curve (Figure 4.7b). Based on this procedure, mean value of k is evaluated as 0.08 for the investigated 9Cr-1Mo steel. By differentiating Eq. (3.16) with respect to temperature, the incremental change in martensite content with a temperature decrease dT can be expressed as

$$dF_{mart} = [-k \exp\{k(T - M_{start})\}]dT \quad (3.19)$$

While single-pass deposition leads to complete transformations, the thermal cycles in multi-layer deposition often result in incomplete transformations when the local temperature does not rise above A_{c3} or does not cool sufficiently below M_{final} . This is particularly significant in multi-layer conditions, where the likelihood of incomplete A→M transformation increases when the M_{start} is relatively low and the inter-pass temperature is comparatively high. As illustrated in Figure 4.8, the multi-pass thermal profile involves three successive

cycles, representing the preceding (N-1), current (N), and subsequent (N+1) layers. In the layer (N+1), this fresh martensite is retained, since the peak temperature of that cycle does not exceed A_{C3} . This subcritical reheating arises because the deposited wall acts as a thermal sink, dissipating heat into the substrate and surrounding layers, while the increasing build height, elevated inter-pass temperature, and reduced energy absorption in solidified layers further limit the temperature rise. Consequently, the N layer undergoes only partial re-austenitization, preventing complete transformation in subsequent cycles. Incomplete M→A transformation occurs at X_a (the first peak between A_{C1} and A_{C3}), while incomplete A→M transformation occurs at X_b (second valley between M_{start} and M_{final}). At X_b , during the cooling of layer n, the transformation is only partial, producing some fresh martensite. In the following layer N+1, this fresh martensite is retained, since the peak temperature of that cycle does not exceed A_{C3} . Consequently, the reheating of a mixed microstructure comprising martensite and austenite can lead to complex phenomena such as rapid carbon partitioning (within <10 s) from supersaturated martensite into the untransformed austenite, similar to what has been reported in quenched and partitioned (Q&P) steels [165]. This carbon enrichment increases the stability of retained austenite and effectively reduces $M_{start} - M_{final}$ temperature window. For simplicity, the current study neglects such intricate microstructural effects. Instead, it is assumed that during cooling of layer N+1, fresh martensite does not nucleate immediately upon reaching M_{start} , due to the presence of pre-existing martensite. To capture this behavior, a threshold temperature for the A→M transformation is defined as

$$T_{sm} = M_s + \frac{1}{k} \ln \left(1 - \frac{F_m}{F_{max}} \right) \quad (3.20)$$

where F_{max} is defined as the sum of the existing fractions of austenite and martensite, representing the maximum martensite fraction that can be generated at a given material point. It should be emphasized that Eq. (3) remains applicable even when the microstructure initially contains only austenite, as in the case of a single-pass cycle shown in Figure 4.8. Under such conditions, $F_m = 0$, and therefore the threshold temperature reduces to $T_s = M_{start}$. The expression for martensite fraction can be reformulated to account for the effect of incomplete A→M transformation as

$$F_m = F_{max} \{1 - \exp [k(M_{start} - T)]\} \quad (3.21)$$

At X_a in Figure 4.8, the heating cycle of layer N-1 leads to an incomplete martensite-to-austenite (M→A) transformation. During the subsequent reheating in layer N, the onset temperature of the M→A transformation is shifted due to the presence of residual austenite. Adopting an approach analogous to that used for the incomplete austenite-to-martensite case, the threshold temperature for the M→A transformation is defined as

$$T_{sa} = A_{C1} + F_a(A_{C3} - A_{C1}) \quad (3.22)$$

The phase transformation-induced volumetric strain is evaluated directly from the temperature-dependent phase fractions by accumulating the incremental contributions of each active pathway. At each temperature step, the change in volumetric strain is equivalent as the sum of per-fraction volumetric increments and is defined by

$$d\varepsilon_{Vol} = V_a dF_a(T) + V_m dF_m(T) \quad (3.23)$$

where $V_a = -2.288 \times 10^{-3}$ contraction for M→A and $V_m = 3.75 \times 10^{-3}$ expansion for A→M are the per-unit-fraction volumetric strain coefficients [166]. The differential dF_a and dF_m are nonzero only within their respective transformation windows ($A_{C1} < T < A_{C3}$ for austenitization and $M_{final} < T < M_{start}$ for martensitic transformation). On integration equation (3.23)

$$\varepsilon_v(T) = \int_{T_0}^T (V_a dF_a + V_m dF_m) = V_a \Delta F_a(T) + V_m \Delta F_m(T) \quad (3.24)$$

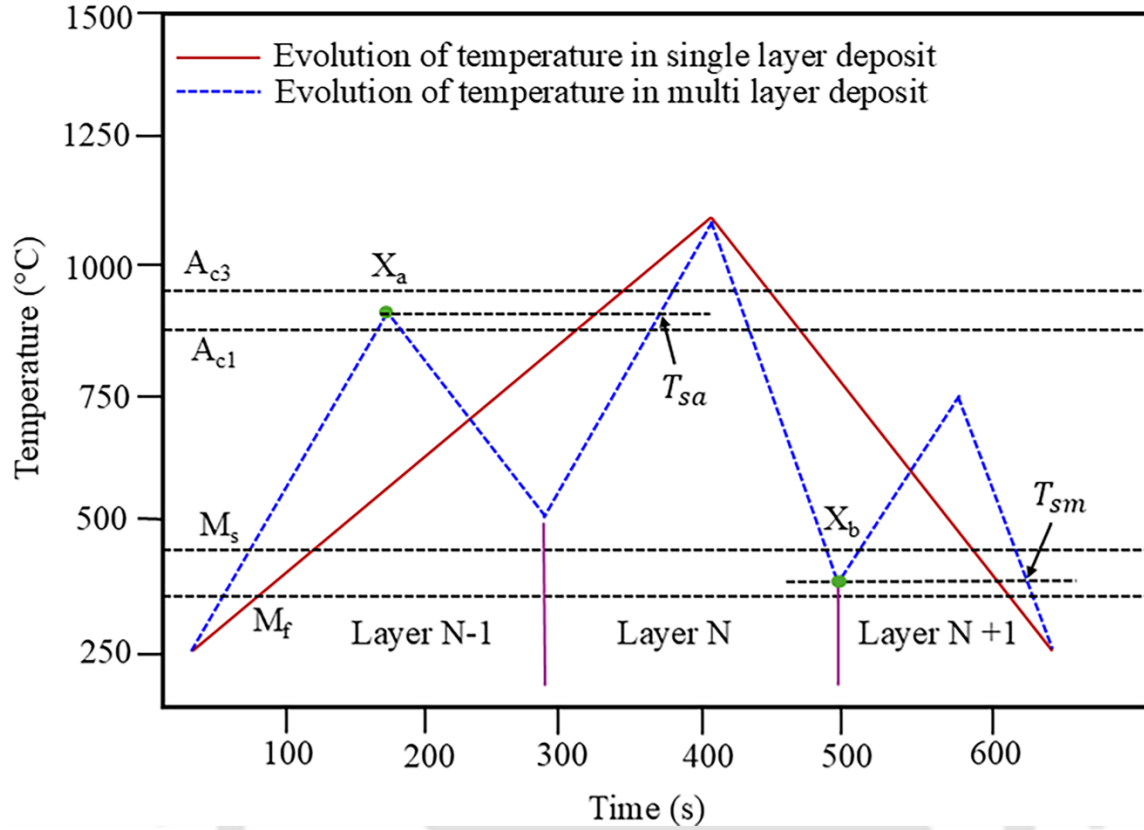


Figure 4.8: Schematic representation of thermal histories illustrating complete and incomplete phase transformations during single-layer and multi-layer deposition.

The martensitic transformation is typically triggered upon cooling below the martensite start temperature (M_s) in materials that have undergone prior austenitization. The transformation results in a progressive increase in the volume fraction of martensite as temperature decreases. When thermal and phase evolution are tracked incrementally, the updated martensite fraction at any given time step can be expressed as

$$F_{mart}^{new} = F_{mart}^{previous} + dF_{mart} \quad (3.25)$$

where F_{mart}^{new} and $F_{mart}^{previous}$ represent the martensite volume fractions at the end and beginning of the increment. In the context of martensitic transformation, the release of latent heat significantly alters the thermal evolution during the cooling phase. The heat generation rate per unit volume due to this transformation [167] is expressed as

$$\dot{Q} = dh_m * \left(\frac{dF_{mart}}{dt} \right) \quad (3.26)$$

where dh_m represents the transformation enthalpy associated with the martensitic phase and is considered as $6.4 \times 10^8 Jm^{-3}$ [168] based on validated thermophysical data. This approach allows the latent heat release to be dynamically coupled to the phase transformation kinetics within a FE framework. The martensite fraction is evaluated at each time increment using the KM model and its temperature derivative, while the local cooling rate provides the time-dependent behaviour. By incorporating this heat generation term into the energy balance equation typically through user-defined (HETVAL) heat source function. This implementation ensures that the exothermic nature of martensitic transformation is physically represented within the thermal model, improving the fidelity of the simulation.

The transformation from austenite to martensite induces a fundamental crystallographic change from FCC to BCC/BCT structure, leading to volumetric expansion, as illustrated in Figure 4.7b. This martensitic transformation (MT) not only refines the microstructure of 9Cr-1Mo steel but also induces substantial alterations in its macro-mechanical properties, including yield strength. Moreover, atomic migration and lattice reconfiguration during the phase transition contribute to phase transformation plasticity, further influencing the material's deformation behavior. As a result, the total strain increment during the cooling phase can be expressed as [169,170]

$$d\varepsilon_{total} = d\varepsilon_E + d\varepsilon_P + d\varepsilon_T + d\varepsilon_{Vol} + d\varepsilon_{Trp} \quad (3.27)$$

where $d\varepsilon_E$, $d\varepsilon_P$, $d\varepsilon_T$, $d\varepsilon_{Vol}$ and $d\varepsilon_{Trp}$ represent increments in elastic strain, plastic strain, thermal strain, volumetric expansion, and phase transformation induced plasticity (TRIP). The effects of solid-state phase transformations is implemented using various user subroutines, as illustrated in Figure 4.9.

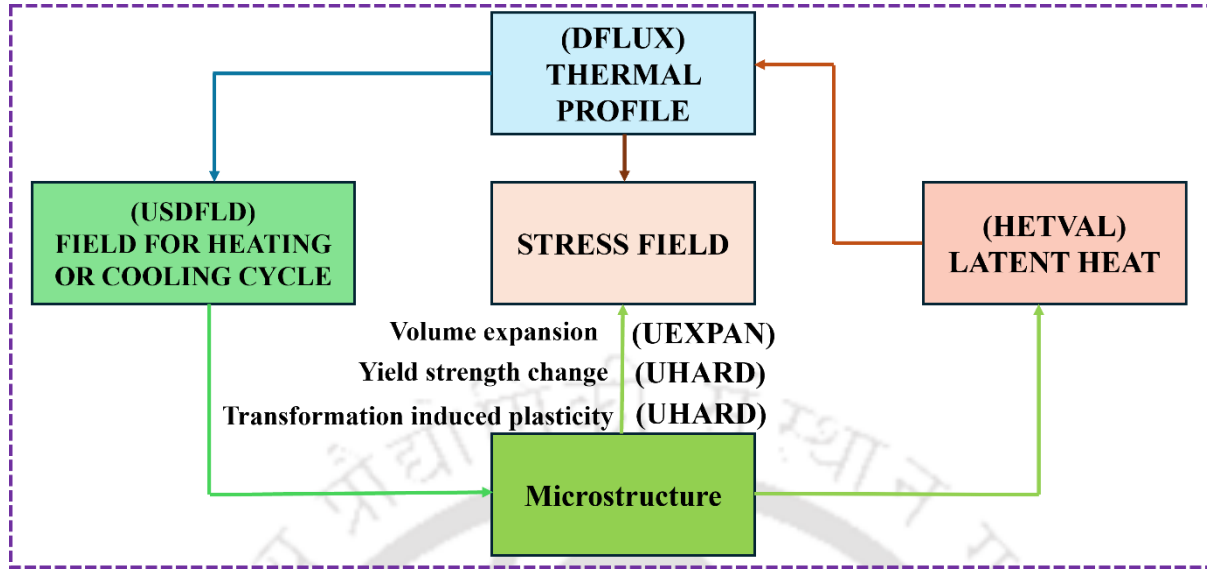


Figure 4.9: Schematic illustration of the computational workflow integrating subroutines for phase transformation-induced residual stress prediction in DED fabricated rectangular component.

Transformation-induced plasticity (TRIP) is a critical deformation mechanism that occurs when SSPT take place under applied stresses. Although the external stress may be well below the yield strength, the transformation process can lead to irreversible strains within the structure. This phenomenon becomes particularly significant in arc-based DED process. Two primary mechanisms contribute to TRIP. The Greenwood–Johnson effect, arises from the volumetric mismatch between the parent and product phases during transformation [29]. This mismatch generates internal stresses at the phase boundaries, which in the presence of external stress, result in additional plastic strain. The second contribution stems from the preferential orientation of martensitic variants under stress, as described by the Magee effect [30]. This mechanism reflects the transformation shear associated with the crystallographic nature of martensite formation and its alignment with the applied stress field. In the context of arc-DED, where rapid thermal gradients and phase changes are inherent, the development of TRIP can significantly affect the residual stress state. To incorporate TRIP effects into continuum-scale simulation, the incremental transformation plasticity strain tensor is modelled as [31]

$$d\varepsilon_{Trp} = 3K_{tp}(1 - F_{mart}^{new})S_{ij}dF_{mart} \quad (3.28)$$

where K_{tp} is the material-specific TRIP coefficient for steel ($4 \times 10^{-12} \text{ MPa}^{-1}$) [117,171]. S_{ij} is the deviatoric stress tensor that dictates the displacive mechanism of martensitic transformation under shear stress only. This formulation captures the stress-induced TRIP strain under the progression of phase transformation and stress field. Multiplicative factor $(1 - F_{mart}^{new})$ ensures that the TRIP contribution diminishes as the transformation approaches completion.

The incremental thermal strain resulting from a change in temperature can be expressed as

$$d\varepsilon_T = \alpha_T dT \quad (3.29)$$

where α_T represents the temperature-dependent coefficient of thermal expansion. Elastic behaviour is described by generalized Hooke's law, where both the Young's modulus and Poisson's ratio are treated as temperature-dependent properties. For the onset of plasticity, the Von Mises yield criterion is employed to define the yield surface, while subsequent plastic flow is governed by the associated Prandtl–Reuss flow rule. This ensures that the plastic strain increment aligns with the direction of the deviatoric stress tensor. The temperature-dependent plastic strain data, corresponding to a strain rate of 0.003 s^{-1} are incorporated from validated experimental studies specific to 9Cr-1Mo ferritic-martensitic steel [158].

To quantitatively correlate phase transformation kinetics with mechanical behavior in the arc-based DED of 9Cr-1Mo steel, a parameter termed the kinetic-mechanical index (K_m) is introduced. This parameter is defined as

$$K_m = \frac{F_{mart} |\Delta\varepsilon_{ptm}|}{M_{start} - M_{final}} \quad (3.30)$$

where $\Delta\varepsilon_{ptm}$ is the transformation-induced strain determined from dilatometric measurements, and $(M_s - M_f)$ denotes the transformation temperature window. The parameter K_m captures the average rate of mechanically effective phase transformation strain per unit temperature, thereby bridging the gap between microstructural transformation dynamics and macroscopic mechanical response. Figure 4.10 depicts this index for different scanning patterns.

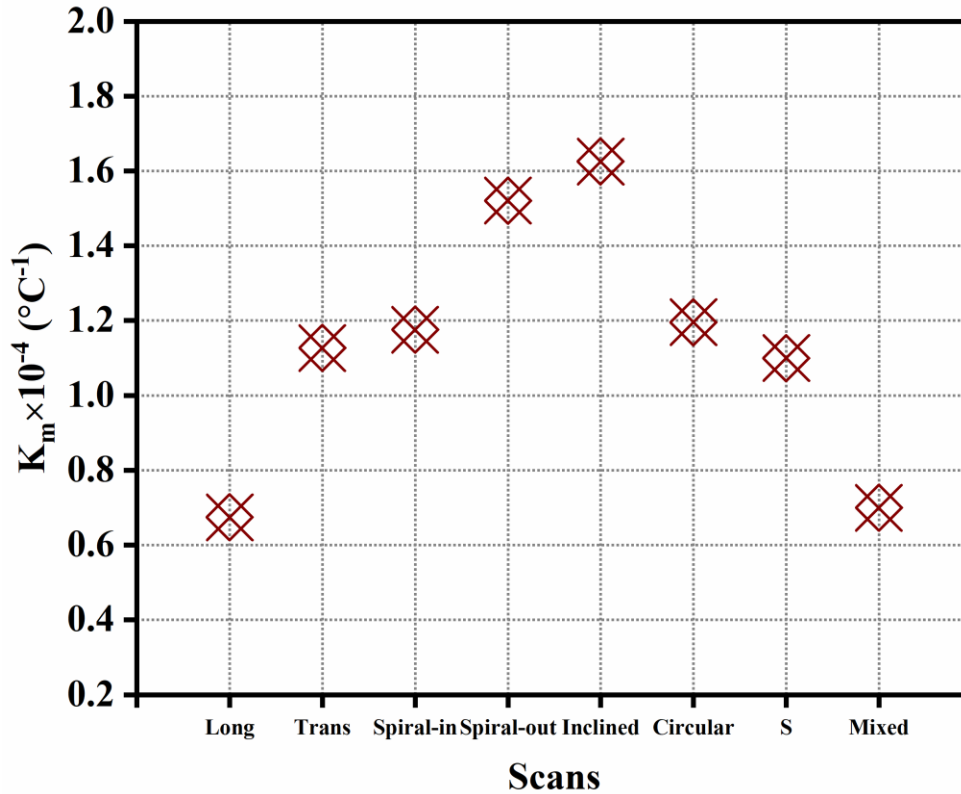


Figure 4.10: Variation of kinetic-mechanical index (K_m) for longitudinal, transverse, spiral in, spiral out, inclined and circular scanning pattern utilized for fabricating rectangular components.

4.6 Artificial intelligence models

Artificial Intelligence (AI), and in particular Machine Learning (ML) and Deep Learning (DL), provide powerful tools to complement experimental and numerical studies of wire-based DED process. By learning complex, nonlinear relationships from data, these models enable accurate prediction of bead geometry, thermal histories, and residual stress fields. In the present study, AI-driven thermo-mechanical modeling is integrated with experiments to tailor residual stress in wire-based DED of ferritic steel, offering a pathway for process optimization and improved component performance.

4.6.1 Forward prediction using AI models

In this framework, the influence of deposition attributes such as power and velocity on transient temperature evolution is first captured using machine learning algorithms of varying

complexity, including KNN, DT, RF, XGBOOST, and ANN. The predictive performance of these models is systematically evaluated against FE-generated datasets, enabling identification of the most accurate models for estimating both transient temperature profiles and peak temperatures under unseen process conditions. Building on this, advanced deep learning architectures such as LSTM, Bi-LSTM, GRU, and TCN are applied to predict the evolution of transient residual stress profiles, leveraging their strength in modeling sequential dependencies. In addition, inter-layer dwell time effects on thermo-mechanical responses are assessed through predictive modeling, encompassing both interpolation and extrapolation scenarios. Together, these AI models provide a forward-prediction framework that bridges process parameters with thermal and mechanical outcomes, offering a computationally efficient alternative to traditional FE simulations.

4.6.1.1 Development of AI models for single track deposits

Non-linear datasets can be handled by using suitable ML algorithms. The generation of data through the experimentally FE model and fitting with appropriate ML algorithms on training datasets to understand the underlying physics involved in melting and solidification of deposits is known as physics-informed machine learning (PIML) model. Sequential steps for the development of PIML models are illustrated in Figure 4.11. Hence, the present work analyzes the prediction of the transient temperature profile (multiple data points) and peak temperature (single data point) for the deposition of single layer using PIML model. The DED process is developed for P91 on SS316L substrate. The simulations are performed by considering the deposition velocity and power as process parameters for 121 different cases. Hence, the dataset contains 33462 rows and four columns (power, velocity, time as a feature, and temperature as output variables) (Figure 4.12). However, for the prediction of peak temperature, time is not considered as a feature. Further, the dataset is split into the training (80%) and testing (20%) parts that contain all the features. The fitting of ML models are performed on the training dataset, and the predicted outputs are compared with the testing dataset.

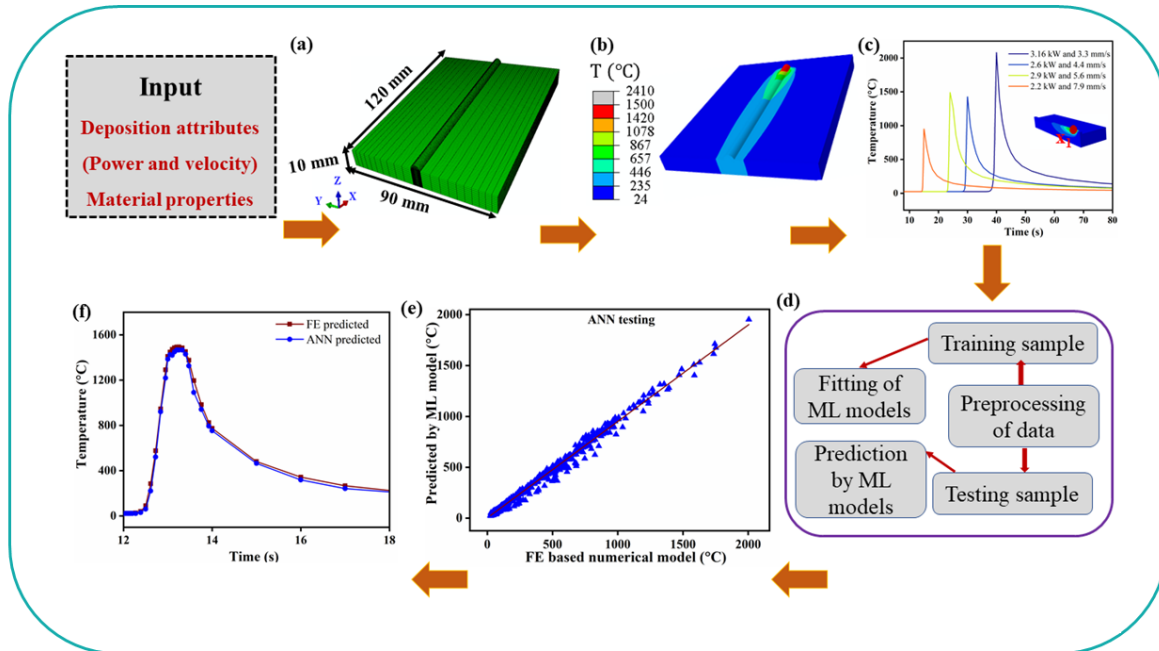


Figure 4.11: Sequential steps involved in digital twin model: (a) Schematic representation of the solution geometry, (b) 3D temperature profile, (c) time-temperature profile at different process parameters, (d) steps involved in integrating with ML algorithms, (e) output predicted by ML algorithm for training, and (f) testing of ML model.

Five different ML algorithms associated with different degrees of non-linearity are fitted to analyze the dataset obtained from a physics-based FE model. Finally, the performance of the models are evaluated and compared in terms of computed error. The models having the highest accuracy are utilized for the prediction of temperature at multiple data points (transient temperature profile) and single data point (peak temperature) at validation attribute. The transient temperature profile during the deposition of material has a significant impact on the microstructure and residual stresses evolution that decides the mechanical properties of the DED component.

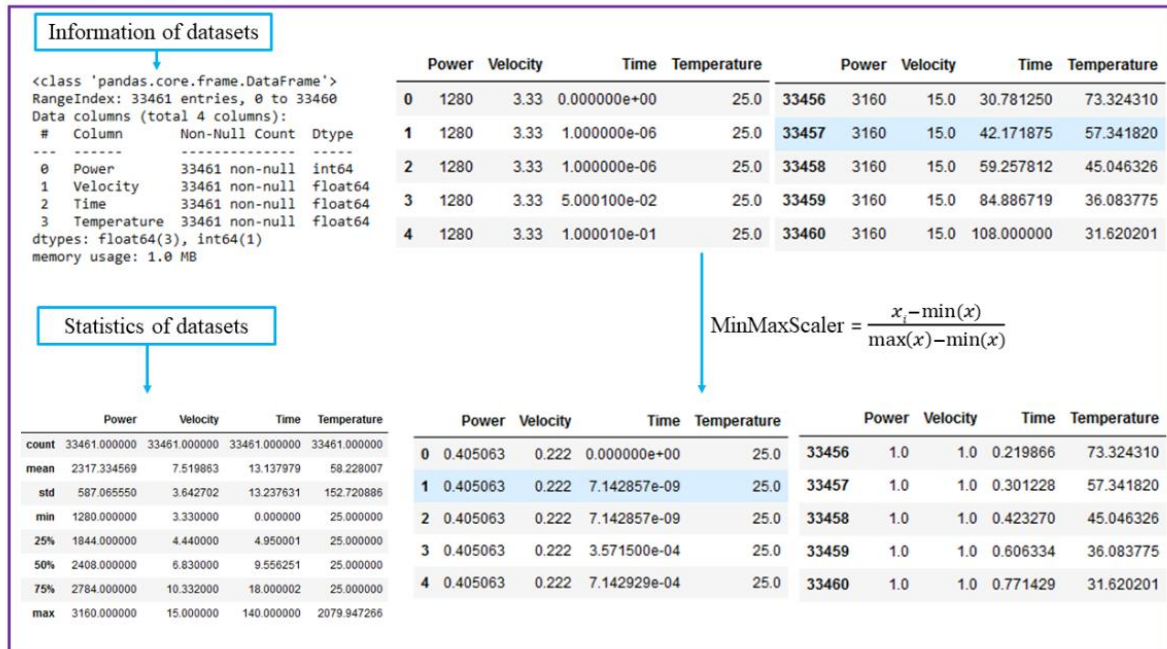


Figure 4.12: Basic information, statistics and preprocessing steps involved for datasets for the prediction of transient thermal profiles.

The pre-processing steps are followed before training the ML model. Over the specified range of power, velocity, and time, the weightage of each feature is mapped with a scale ranging from 0 to 1. In the present analysis, five supervised ML models such as Artificial neural network (ANN), Extreme Gradient Boosting (XGB), K-nearest neighbors (KNN), Decision Tree (DT), and Random Forest (RF) are applied to identify the most efficient one for evaluating transient temperature profile. All these models are developed using the open-source library (sci-kit-learn in Python) [172]. A DT model consists of tree-like structures with roots, branches, leaves, and nodes, and it is more efficient for data points with non-linearity [173]. However, DT generally undergoes overfitting that can be overcome by the RF model. RF is an ensemble learning technique that adopts a bagging methodology coupled with the decision of multiple trees [174]. XGB model is generally applied for regression problems where the requirement of accuracy is more [175]. KNN model is based on the concept of evaluation of euclidean distance and groups the output of similar features together and provides the mean value [176]. ANN model has the capability of identifying the complex relationship among the non-linear data points during training [177]. The basic architecture of the ANN model consisting of input layers, hidden layers, and output layers is shown in Figure 4.13. The hidden

layers contain the number of neurons having a weight and bias to get higher accuracy by adjusting the errors in each epoch, called back-propagation technique. Neurons comprise transfer and activation functions [178]. In the current study, the number of hidden layers are considered as three, the number of neurons in each layer is thirty-five, and the number of epochs are six thousand. The activation functions used in the input and output layers are relu and linear whereas, only relu is used in the three hidden layers.

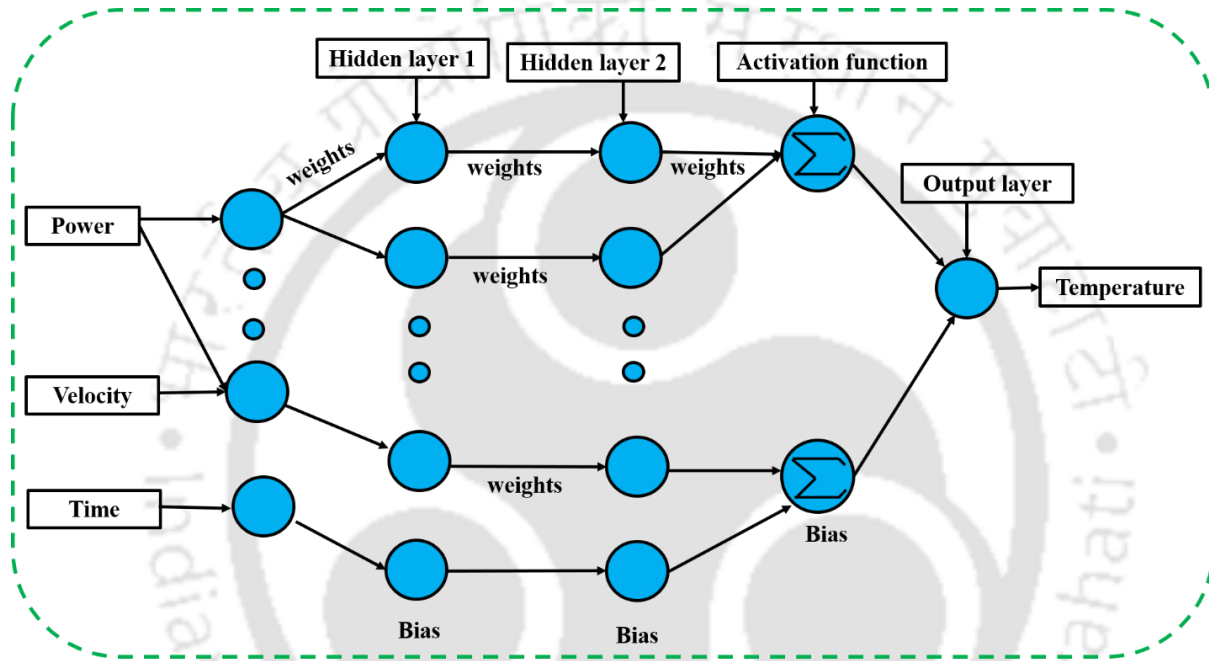


Figure 4.13: Architecture of the ANN model utilized for the prediction of the transient thermal profiles in the study.

Although substantial progress has been made in modeling residual stress during DED process, only a few studies have systematically explored the effectiveness of temporal DL models. Evolution of residual stress is highly transient, governed by complex thermal and mechanical interactions during deposition of every layer. This demands use of models capable of accurately learning from time-dependent data. In this work, we investigate four distinct sequence learning architectures: LSTM, BiLSTM, GRU, and TCN. These models are well suited for capturing temporal dynamics relevant to stress generation. LSTM, BiLSTM, and GRU leverage memory-based gating mechanisms to model stress accumulation over time, while TCN employs dilated convolutions to learn long-range dependencies. The results of the

present study, based on the time series data generated from experimentally validated finite element simulations, show that TCN delivers the highest accuracy by effectively capturing complex, multiscale patterns in stress evolution, making it the most suitable architecture for this task.

Figure 4.14 illustrates the architectures of the DL models used for residual stress prediction. LSTM networks capture long-term dependencies in sequential data through memory cells regulated by input, output, and forget gates [179] (Figure 4.14 a). BiLSTM enhance prediction accuracy by processing input sequences in both forward and backward directions, providing richer temporal context [180] (Figure 4.14 b). GRU streamlines the architecture of LSTM by unifying the input and forget gates into a single update gate and integrating the hidden and cell states, offering a balance between accuracy and computational efficiency [181] (Figure 4.14 c). TCNs replace recurrent architectures with convolutional layers, leveraging causal and dilated convolutions to effectively capture both short and long-range temporal dependencies while ensuring stable training and high computational efficiency [182]. LSTM, GRU, BiLSTM, and TCN models are implemented using TensorFlow library and trained for up to 5000 epochs with early stopping based on validation loss. GRU and BiLSTM consisted of a single recurrent layer with 64 units followed by a dense output layer. GRU captures temporal dependencies through gated updates while BiLSTM processes sequences in both forward and backward directions for richer context. The TCN model uses stacked 1D convolutional layers with causal and dilated convolutions, employing a dilation rate sequence of 1, 2 and 4 to expand the receptive field (Figure 4.14 d). All models used ReLU activation in hidden layers and the Adam optimizer to minimize root mean square error (RMSE).

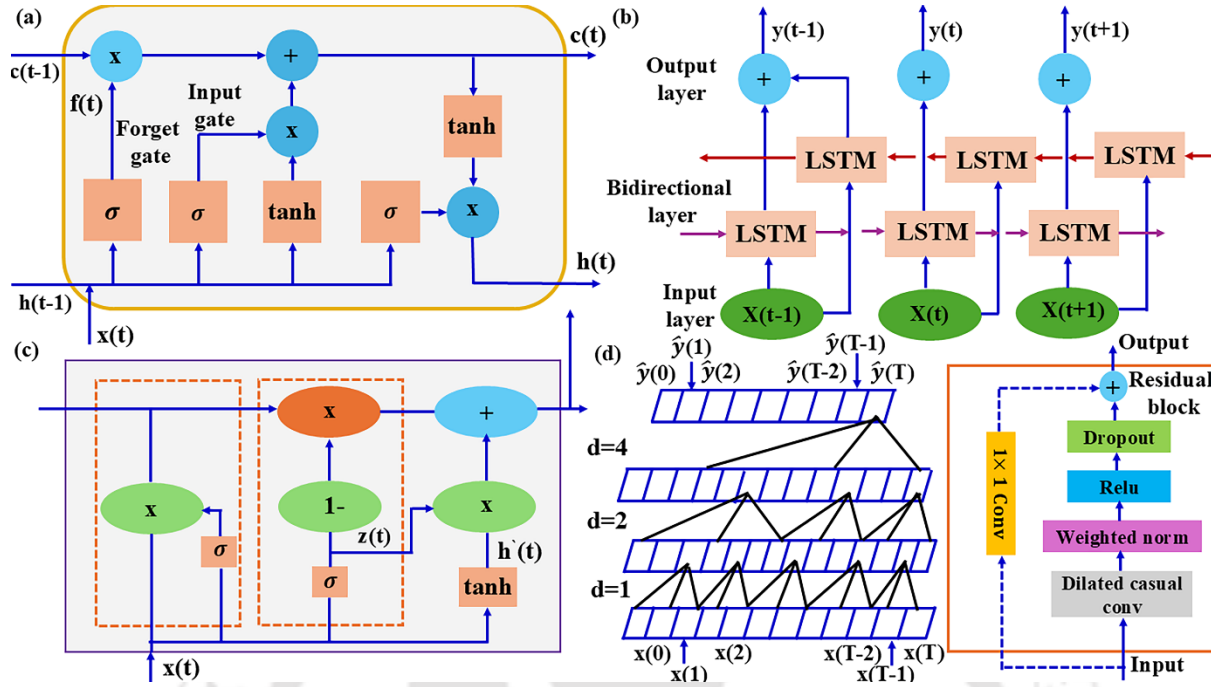


Figure 4.14: Architecture of the RNN based models utilized for the prediction of transient residual stress: (a) LSTM, (b) Bi-LSTM, (c) GRU and (d) TCN model.

4.6.1.2 Development of AI models for single track multi-layer deposits

In the present work, ANN is considered as deep learning model where back-propagation algorithm is employed to capture the non-linear behavior of data set. Initially, a random weight is assigned to the neurons. Subsequently, the weighted sum of the input datasets along with the bias is evaluated using transfer function and passed to the hidden layers. An activation function is defined to check the output of transfer function. If these values are passed by activation function, the error between the actual and predicted values are measured by loss function. Based on the value of the loss function, all weights are adjusted to reduce the error until convergence criteria are met. For training of ANN model, rectified linear unit (ReLU) is utilized in input and hidden layers due to its rapid convergence and unique capability of addressing gradient vanishing problem [183]. However, linear activation function is utilized for output layer. The optimal hyperparameters consisting of number of hidden layers and neurons in hidden layers, learning rate and batch size are evaluated to enhance the learning and prediction efficacy of the ANN model. The optimal number of neurons in each hidden layer is obtained using grid search algorithm. The learning rate and batch size are 0.0001 and 5, respectively in the training phase. Out of total datasets generated, 90% are randomly selected

for training and remain utilized for validation purposes for the cases of temperature, residual stress and inter-layer dwell times. Further, the prediction efficacy of ANN model is performed for interpolation set (180s, 270s), which is within the experimental range. While the extrapolation data set (450s, 500s) is considered outside the range.

The architecture of DL model is depicted in Figure 4.15 that consists of input, hidden and output layers and optimizer (Adam). In the present analysis, the errors between training and testing sets are minimized by enhancing the number of hidden layers as well as number of neurons in a hidden layer. The dynamic architecture of the hidden layer is depicted in Table 4.4. The number of epochs considered while fitting a model is five thousand. The distribution of datasets for training, testing and validation is depicted in Table 4.5. The accuracy of the models is checked using evaluation metrics. The coefficient of determination (R^2) and root mean square error (RMSE) are the measure of model quality. The mathematical expression for these evaluation metrics is given as

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} \quad (3.31)$$

$$RMSE = \sqrt{\frac{\sum(y_i - \hat{y}_i)^2}{n}} \quad (3.32)$$

where y_i and $\hat{y}_i$ are the actual and predicted values; $\bar{y}$ illustrates the average value of temperature and residual stress.

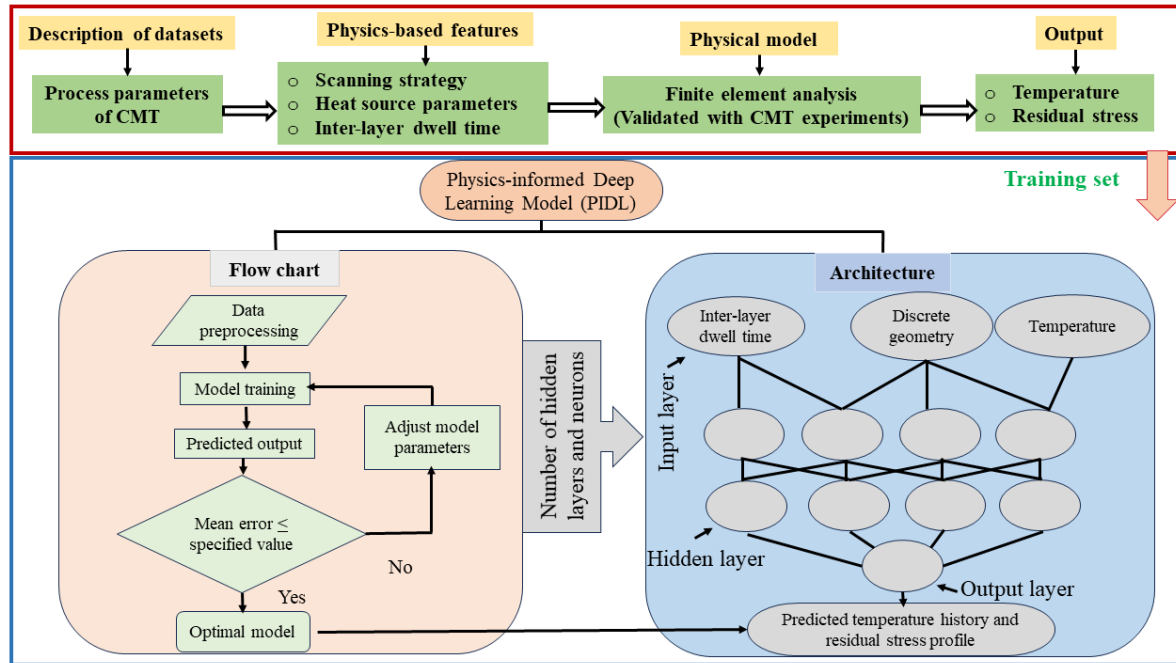


Figure 4.15: Methodology utilized for imparting physical domain information of multi-layer DED process for the prediction of thermal and residual stress evolution.

Table 4.4: Architecture of DL models with varying numbers of neurons.

Models	Number of neurons in the hidden layer					Total neurons
	1 st layer	2 nd layer	3 rd layer	4 th layer	5 th layer	
Model-1	80	-	-	-	-	80
Model-2	80	60	-	-	-	140
Model-3	80	60	40	-	-	180
Model-4	80	60	40	20	-	200
Model-5	80	60	40	20	10	210

Table 4.5: The datasets used in the present bi-directional PIDL model.

Dataset	Inter-layer dwell time (s)
---------	----------------------------

Training sets	100, 125, 150, 175, 200, 225, 250, 275, 300, 325, 350, 375, 400
Interpolation test set	180, 270
Extrapolation test set	450, 500

4.6.1.3 Development of AI models for multi- track-multi-layer deposits

The architecture of the TCN model constructed for modelling the dilatometric response of 9Cr1Mo steel during the DED process is illustrated in Figure 4.16. This deep learning framework is designed to predict transformation-induced strain by leveraging the temporal evolution of thermal and geometric process variables encountered during AM cycle. Attributes to the model is a multivariate time-series comprising four critical features: deposition time, deposition pattern, powder feed angle, peak temperature, and the secondary thermocouple temperature (TC2), which collectively capture the thermal gradient and spatial orientation effects inherent to DED. These features are segmented into overlapping windows of 20-time steps, enabling the model to retain a temporally contextualized memory of both recent and earlier thermal histories critical to martensitic phase transformation. To learn temporal dependencies across varying temporal scales, the network implements a series of one-dimensional causal convolutional layers with exponentially increasing dilation rates ($d = 1, 2, 4, 8, 16, 32$) and a fixed kernel size of 6. The causal structure ensures that predictions at any time step rely solely on current and preceding inputs, which is essential for preserving the causal integrity of physical phenomena in thermal processing [53]. This dilated design significantly expands the receptive field, allowing the network to simultaneously model short-term thermal fluctuations and long-range dependencies, which are pivotal in capturing the onset and kinetics of solid-state transformations.

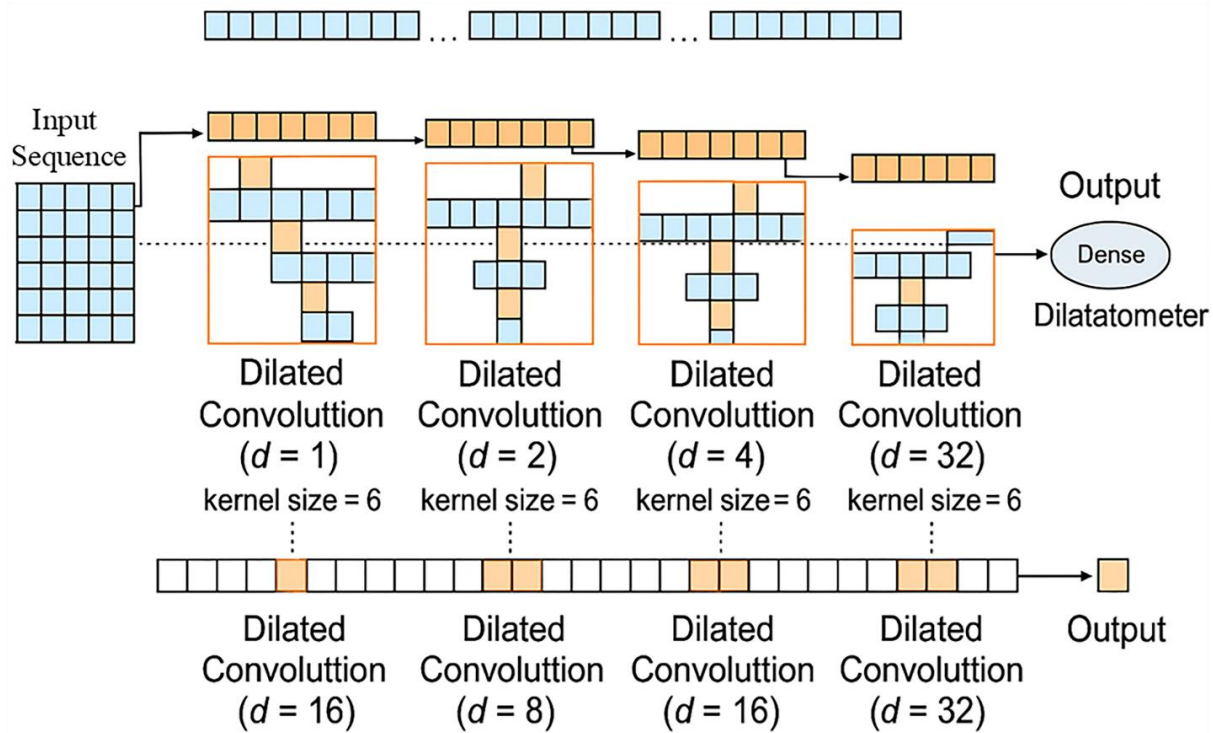


Figure 4.16: Schematic representation of the TCN architecture employed for time-series prediction of dilatometric strain in 9Cr-1Mo steel.

Each convolutional layer is followed internally by a ReLU activation function and dropout layers that aid in non-linearity and regularization [184]. The final representation is fed into a fully connected dense layer, producing a single scalar output representing the predicted dilatometric strain for the terminal time step in each sequence window. This output encapsulates the accumulated strain arising from thermal expansion, contraction, and phase transformation, specifically martensitic formation, which governs residual stress development in ferritic-martensitic steels. TCN network is trained using the Adam optimizer with root mean squared error (RMSE) as loss function. A batch size of 32 and a training duration of 30 epochs are employed. A validation split of 20 percent ensured early detection of overfitting. Throughout training, the model effectively minimized error and maintained convergence, validating its capability to generalize across unseen temporal profiles.

4.6.2 Backward prediction using AI models

While forward prediction establishes the link between process parameters and resulting thermo-mechanical responses, an equally important challenge lies in the inverse design of deposition attributes to achieve desired outcomes. In wire-based DED of 9Cr-1Mo steel, backward prediction provides a data-driven route for tailoring process settings based on targeted thermal and stress responses. For single-track deposits, peak temperature is selected as a key target variable since it governs molten pool dimensions, cooling rates, and solidification kinetics, which in turn strongly influence residual stress evolution. By using AI models, process parameters such as power and velocity are inversely predicted from these targeted peak temperatures. Effectively mapping thermal requirements back to controllable deposition inputs. This is particularly significant as both power and velocity directly regulate heat input and, consequently, the peak temperature. Beyond thermal considerations, backward prediction is extended to residual stress control, where inter-layer dwell times are inversely estimated from desired stress levels typically constrained to remain below the yield strength in thin-wall structures.

4.6.2.1 AI models for the prediction of deposition attributes for single track

In single-track deposition, accurate estimation of process parameters from targeted thermal responses is essential for controlling molten pool behavior as it regulates microstructural and residual stress evolution. AI models such as ANN and XGBOOST are employed to perform this inverse prediction of deposition attributes. As these two models are performed quite well on forward prediction of peak temperatures. Hence, these two models are further optimized for backward prediction. Sequential steps adopted for this task are illustrated in Figure 4.17. The framework first considers velocity and temperature as input features to predict the required power, establishing the direct role of heat input in regulating peak thermal fields. In a complementary approach, power and temperature are utilized as features to estimate velocity, thereby completing the mapping between process parameters and thermal responses. Through this dual strategy, the models enable robust prediction of deposition attributes from targeted peak temperatures, offering a computationally efficient pathway for process design and optimization in directed energy deposition.

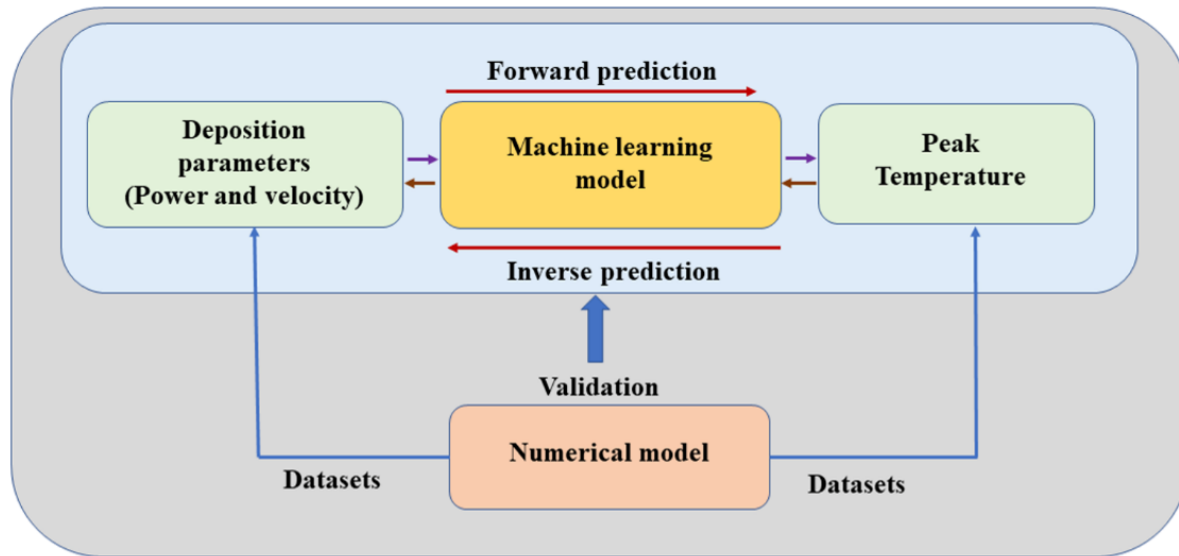


Figure: 4.17: Illustration of the methodology adopted for the forward and inverse prediction using machine learning models for the peak temperature datasets.

4.6.2.2 AI models for the prediction of deposition attributes for multi-layer deposits

In multi-layer deposits, the control of inter-layer dwell time and inter-pass temperature is critical for managing residual stress accumulation and maintaining structural integrity. To achieve this, inverse predictions of these process parameters are performed using DL models trained on datasets derived from both numerical simulations and experimental measurements. The model architecture and training features are illustrated in Figure 4.18. For temperature prediction, dwell time and spatial coordinates are used as inputs, capturing the thermal history across the build geometry. Conversely, for dwell time prediction, key attributes such as residual stress, nodal temperature, and build-direction distance are employed, directly linking thermo-mechanical responses with process settings. Residual stress values are carefully chosen to remain below the permissible tensile strength of 9Cr-1Mo steel, ensuring safe operation during thin-wall fabrication, and are further validated against experimental measurements. Five DL models with varying architectural configurations (Models 1–5) are trained and evaluated. Their performance is assessed by the accuracy of predicted inter-pass temperatures and dwell times under different stress conditions. By integrating material properties, build-direction coordinates, and residual stress thresholds into the learning framework, these models not only enhance predictive accuracy but also ensure that the outputs remain within safe operational limits. This approach provides a reliable pathway for optimizing dwell strategies

in multi-layer builds, reducing the risk of distortion and premature failure. Detailed algorithms utilized for bi-directional prediction are depicted below

Algorithm for developing DL model for bi-directional prediction

Step 1: Generate experimental data of thermal and residual stress

Step 2: Development of FE based thermo-mechanical model

Step 2.1: Calibration of the heat source parameters, convective, radiative heat transfer coefficient; Imposing the movement of deposits using different clamping strategies

Step 2.2: Setting of the threshold value for thermal and residual stress error for comparison

Step 2.3: Validation of the thermo-mechanical model with experimental results

if error > threshold value **do**

Back to step 2.1 and again calibrate the model

else

A physics-based numerical model is ready for thermal and residual stress evaluation at different levels of dwell times

end if

Step 3: Adequacy in training and validation datasets for imparting the physical basis of the DED process

Step 3.1: Establishment of varying training sample size and architecture of the DL model

Step 3.2: The performance of DL models is checked using evaluation metrics (R^2 , RMSE)

Step 3.3: Set the threshold limit of RMSE

if error > threshold limit **do**

Back to step 3.1

else

Compute the non-linear thermal and residual stress profile along with prediction timing on the interpolated and extrapolated dwell sets and compare with experiments

end if

Step 4: Modify features of datasets by considering residual stress below the yield strength of P91 material for the prediction of inter-layer dwell times.

Step 4.1: Modifying the training sample size and architecture of DL model

Step 4.2: Set the permissible value of error

if error > permissible limit **do**

 Back to step 4.1

else

 Compute the inter-layer dwell times in different layers with prediction timing

end if

Step 5: PIDL model is ready for bi-directional prediction

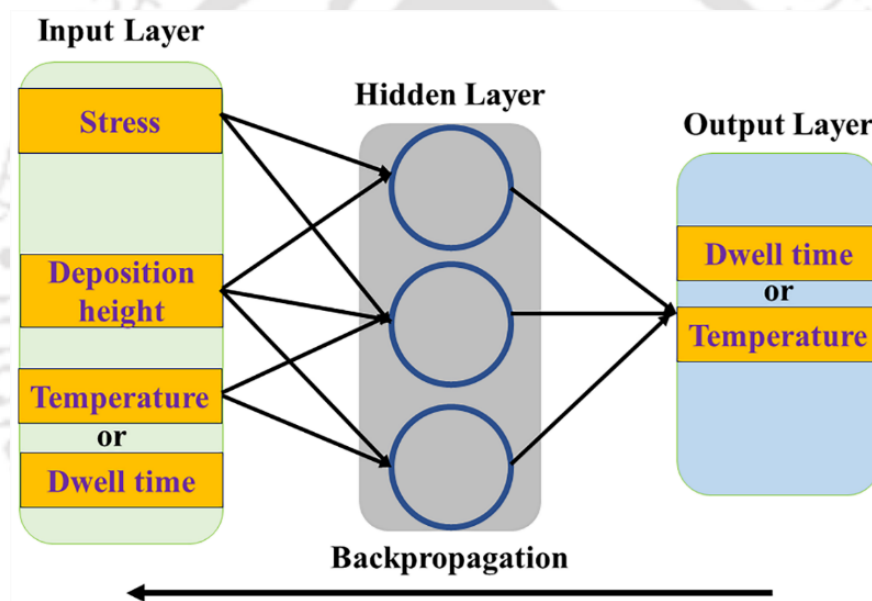


Figure 4.18: Architecture of the deep learning model utilized for inverse prediction of dwell time and temperatures from targeted value of residual stress along the build direction of printed wall for DED process.

4.7 Summary

A comprehensive FE framework is developed to simulate single-track, multi-layer, and multi-track-multi-layer pattern depositions in wire-based CMT-DED of ferritic steels. The thermal model implemented a double-ellipsoidal heat source calibrated against single-bead experiments. While the deposition process is simulated through element birth–death activation governed by Python/Fortran subroutines. Sequentially coupled thermo-mechanical analysis

captured transient heat transfer, molten pool evolution, and stress development. Further, to analyze the effect of phase transformation kinetics driven from various scan patterns, TMM model is developed. To reduce the cost of high-fidelity FE models, PIML approaches are introduced. Datasets generated from validated FE simulations of single-track and multi-layer deposits are used to train AI models capable of capturing nonlinearities in melting and solidification. LSTM, BiLSTM, and GRU networks are fitted on transient residual stress sequential data. TCN model is also trained on this ordinal nature of datasets as it leveraged dilated convolutions to capture both short- and long-range dependencies with stable training. ANNs trained using back-propagation and optimized through grid search, are deployed for predicting inter-layer dwell time responses, inter-pass temperatures and residual stress. Hyperparameter tuning (neurons, layers, batch size, learning rate) and early stopping ensured convergence and minimized overfitting. This integrated FE–AI framework demonstrated high predictive fidelity, with evaluation metrics such as R^2 and RMSE confirming accuracy close to unity. By combining mechanistic insight from calibrated FE models with the efficiency of AI-driven predictions, the approach enables robust forecasting of thermal fields, residual stress distribution, and transformation-induced strain. Importantly, it provides a scalable pathway for tailoring deposition attributes, optimizing dwell times, and mitigating residual stresses in wire-based DED of ferritic steels, offering a balance between physical accuracy and computational efficiency.



Results and Discussions

5.1 General Background

Wire based DED of ferritic/martensitic steels, particularly 9Cr-1Mo, involves highly transient thermal and microstructural evolution that govern residual stress development and mechanical performance. Influence and in-situ monitoring of deposition attributes on these physical phenomena remains challenging. Although FE based numerical models well-established. But these models are computationally intensive when applied across a wide parameter space. To address this, AI frameworks have emerged as efficient surrogates, trained on datasets generated from experimentally validated FE simulations, enabling accurate prediction of transient temperature and residual stress profiles during single- and multi-layer deposition. TCN have shown superior capability in capturing the time-dependent stress evolution, while physics-informed DL (PIDL) models not only replicate nonlinear thermo-mechanical responses at a fraction of the computational cost but also perform inverse predictions, such as identifying optimal inter-layer dwell times (D_{TM}) for stress mitigation. The influence of D_{TM} is especially significant in thin-wall structures where successive reheating and cooling cycles alter the balance between austenite formation and martensitic transformation, thereby dictating residual stress magnitudes. Coupling FE-based TMM models with DL architecture accelerates the exploration of this parameter, ensuring physically interpretable and computationally efficient optimization. Complementing dwell-time control, scanning strategies such as bi-directional deposition reduce tensile residual stress. To deepen our understanding of these interactions, the study employs thermodynamic modelling to

analyse key phase transformations, including martensite stabilization and δ -ferrite dissolution, under the non-equilibrium conditions of the DED process. Microstructural analysis, particularly via TEM, confirms that these optimized strategies refine martensitic laths, reduce dislocation density, and enhance precipitate stability, thereby mitigating Type IV cracking risks. Extending this approach, advanced deposition patterns including spiral, circular, inclined, and mixed strategies actively tailor martensitic kinetics and redistribute residual stress, as revealed through integrated dilatometry, mechanical testing, and FE-TMM simulations. Collectively, the fusion of physics-informed ML/DL models, optimized dwell-time regimes, and scanning strategies establishes a holistic framework that not only accelerates computational predictions but also delivers experimentally validated insights for microstructural refinement, residual stress management, and performance enhancement of 9Cr-1Mo steel in DED, ultimately enabling its reliable deployment in high-performance structural applications.

5.2 AI driven thermo-mechanical analysis of single-track deposits

Single-track-single-layer (STSL) deposits provide a controlled setting to study melt-pool dynamics and the ensuing stress state without the confounding effects of multi-layer reheating. Yet, in-situ sensing is cumbersome and high FE analysis, while reliable, is computationally intensive across broad process windows. To address this, we adopt a PIML route that learns from an experimentally validated FE model to predict both the transient temperature history (multiple time points) and the peak temperature (single point) for 9Cr-1Mo deposits. Five ML algorithms spanning different nonlinear capacities are fitted and compared via standard evaluation metrics. The best performers are then used for temperature prediction at validation attributes. Residual stress in STSL evolves strongly with respect to time driven by transient thermal profiles, steep thermal gradients and martensitic transformation during cooling. Hence, to capture these physical phenomena that are ordinal in nature, sequence models are essential. We therefore evaluate four temporal deep-learning architectures (LSTM, BiLSTM, GRU, and TCN): the gated recurrent models capture stress accumulation through memory mechanisms, whereas the TCN leverages dilated convolutions to learn long-range, multiscale dependencies along the deposition timeline. Using time-series data generated from the validated FE simulations, the TCN achieves the highest accuracy, indicating superior fidelity in mapping

the thermo-mechanical coupling that governs stress evolution in single-track deposits. Collectively, the PIML framework for thermal fields and the TCN-based stress surrogate deliver a fast, accurate, and physically grounded toolkit for AI-driven thermo-mechanical analysis of STSL DED, enabling rapid exploration and optimization of deposition attributes.

5.2.1 Experimental validation of thermal profiles

ML prediction relies on the correctness of FE results. Hence, the thermal model is validated with the experimentally measured temperature at selected thermocouple points. Figure 2(c-d) depicts the transient temperature distribution of deposits at thermocouple points Y1 and Y2. The numerically computed temperature is close to the experimental measurement. The temperature increases first and reaches to a peak point, and gradually decreases when the consumable wire is away from the thermocouple point. The maximum temperature at Y2 is more than that of Y1 since the thermocouple point is closer to the molten pool, and the arc power utilized for the first case is more than that of the second case (2.2 kW and 2.8 kW). The variation of peak temperature with respect to power and velocity is depicted in Figure 5.1(e-f). The weld bead profile is also measured experimentally and compared with the numerically obtained profile (Figure 5.2). The deposited track is assumed as parabolic in nature. Hence, the geometric profile of track is predefined by maintaining the volume flow rate of the process. The similar kind of parabolic profile is also observed from experimental measurement. The peak temperature increases with enhancing power while it reduces on increasing the velocity at any step time. When the deposition speed is low, the concentrated heat source remains close to the molten pool, and it can effectively complement the dissipated heat that leads to a higher temperature. At the increased deposition speed, the heat dissipation is faster, and the elongated molten pool leads to a decrease in peak temperature. Figure 5.2 represents the cross-sectional view of the deposited bead at high and low heat inputs (240 J/mm and 490 J/mm). Both the profile and the dimension of the simulated result are well agreed with the experimentally obtained macrograph.

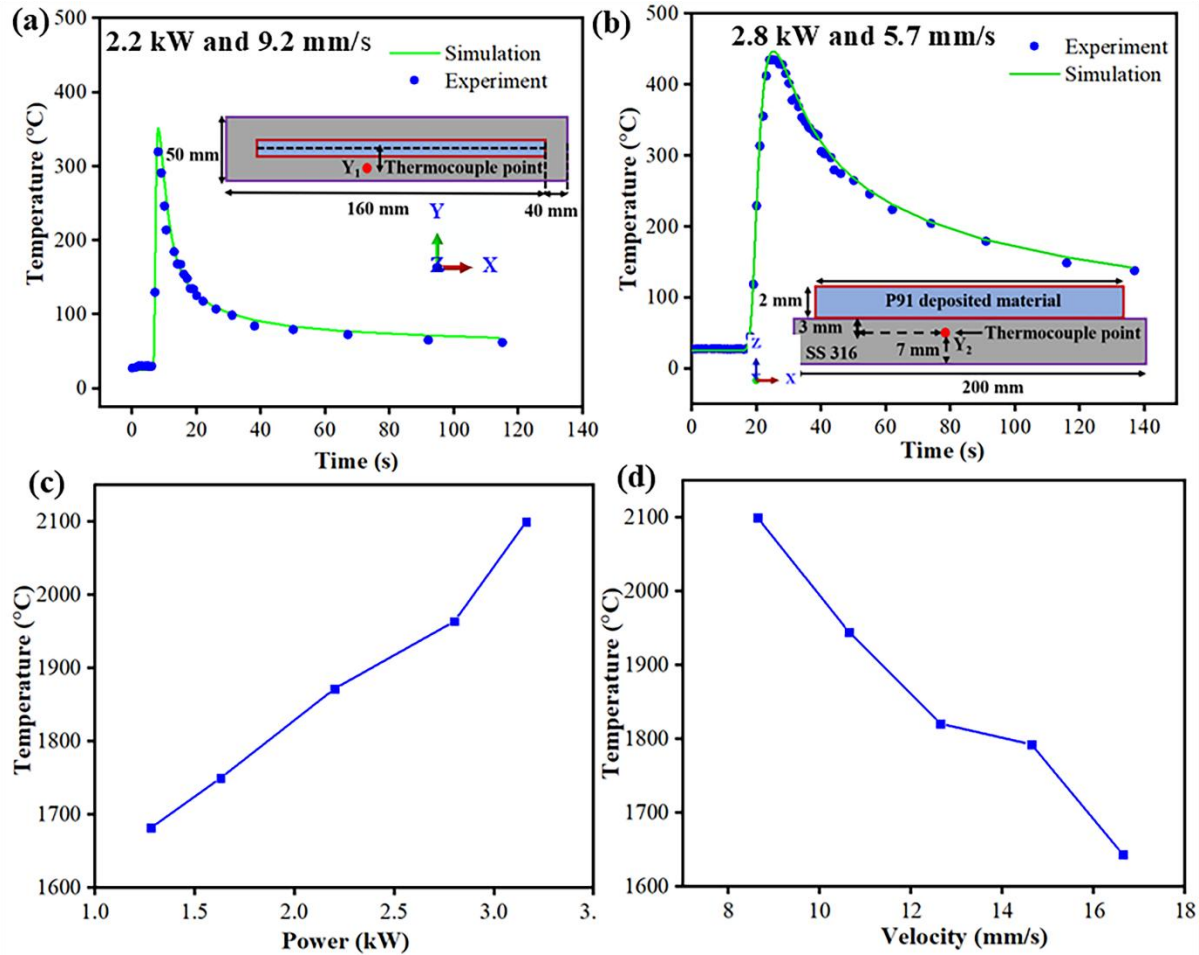


Figure 5.1: (a, b) Comparison between the simulated transient thermal profiles with experimentally measured data at thermocouple points Y₁ and Y₂; Variation of peak temperature at the end of deposition for investigated range of (c) arc power and (d) velocity.

The temperature between 867°C and 920°C (AC_1 and AC_3) illustrates the austenitization temperature range that depicts the transformation of deposits from tempered martensite to austenite. The difference between the solidus and liquidus temperatures of ferritic steel (80°C) is depicted in red color. However, the mushy zone is found wider at the trailing edge for higher deposition speed. With a high degree of constitutional supercooling, this may promote equiaxed grain size. The molten pool is represented by grey color in the ellipsoidal shape. It is obvious that the depth of the molten pool of the deposited material with higher arc power is more than that of the lower one (increased by 29%). However, the 26.3% increase in length attributed to higher deposition speed leads to more heat dissipation. It is obvious that the

developed thermal model can be used to generate several other data that are not possible to measure directly from a simple experimental set-up. The datasets generated utilized for training and testing of a model are considered in the range of 1.28 kW to 3.16 kW arc power and deposition velocity between 3.3 mm/s to 15 mm/s at eleven different levels.

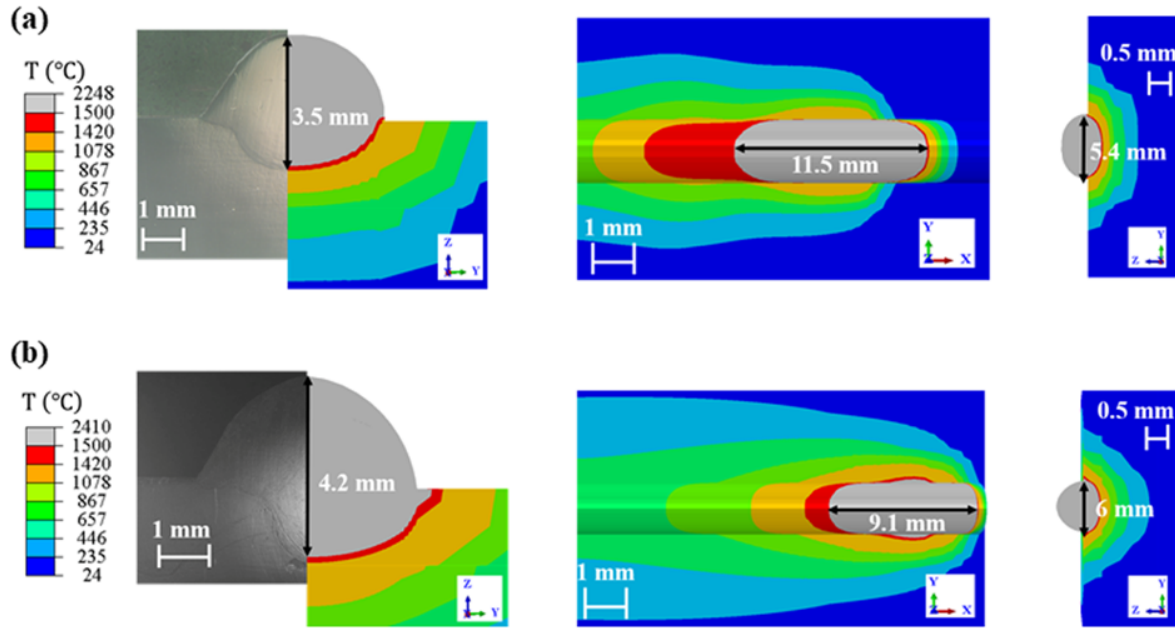


Figure 5.2: Comparison between computed and experimentally measured thermal profile: (b) at an arc power of 2.2 kW and 9.2 mm/s and (c) 2.8 kW and 5.7 mm/s.

5.2.2 Prediction of the transient thermal profiles

Each ML model is hyper-tuned for a given range of hyperparameters in order to get the best R^2 score. The range of parameters used in the present investigation is depicted in Table 5.1. The results from ML algorithms are compared with FE results, and accordingly, the performance of the models are evaluated. Further, the correlation matrix for both the transient temperature distribution and peak temperature are analyzed to know the dependency between features and output variables. Figure 5.3(a) indicates that the accuracy of the RF, ANN, XGBOOST, and DT models are close to 100% while the accuracy for the KNN model is the lowest (88%) for this particular non-linear dataset. All the models are free from the most common issue (underfitting and overfitting), as the difference between the accuracy on training and testing datasets is less than 10%. After fitting a model, an error between the actual and predicted value of temperatures are evaluated using the RMSE metrics (Figure 5.3b).

Computed errors between training and testing data for all the models are less than 16°C for the prediction of transient thermal profile. The difference in RMSE values of ANN and XGBOOST models is less than 4°C followed by RF (9°C), DT (15°C), and KNN (16 °C).

Table 5.1 : Hyperparameters utilized while training a model in order to get the best R^2 score for the predictions.

Models	Hyperparameters utilized for model	Parameters
DT	Criterion	MSE
	Maximum depth	2-7
	Minimum number of split	2-5
	Minimum samples leaf	1-3
RF	Criterion	MSE
	Maximum depth	2-7
	Number of estimators	7-100
	Random state	21
XGBOOST	Maximum depth	2-7
	Number of estimators	7-100
	Learning rate	0.300000012
	Maximum bin	256
ANN	Activation function	Relu
	No of hidden layers	02
	Optimizer	Adam
	Loss	MSE
KNN	Number of neighbors	2-5

Figure 5.4 depicts the accuracy of both the training and testing datasets for all the models to predict the temperature at multiple data points. The predicted data points are closer to the diagonal line, which indicates the degree of accuracy for a particular model (R^2 closer to 1).

First model comprises of low loss (ANN, XGBOOST, RF, DT, KNN) between the actual and predicted value. The data points of all these models are closer to the diagonal line (Figures 5.4(a-h)). It depicts the reliability of the ML models. Figures 5.4(i-j) indicate that the data points for the KNN models are scattered and away from the diagonal line (95% accurate on training and 88% on testing). Overall, the performance of the ANN model is better and it is suited for non-linear data points in the present case. Hence, the ANN algorithm is further utilized for predicting the distribution of transient temperature profile at validation deposition attributes by considering two different heat input levels (155 J/mm and 185 J/mm) (Figure 5.5). These levels of validation attributes are considered outside the process parameter range so that the predicted output by ML models are compared with FE model at the same attributes. ANN algorithm is also capable to consider the effect of changing the deposition attributes of power for the same deposition speed (9.7 mm/s) on changing heat input. The peak temperature difference of 188°C is observed for ferritic steel (P91) deposits on increasing arc power from 1.5 kW to 1.8 kW.

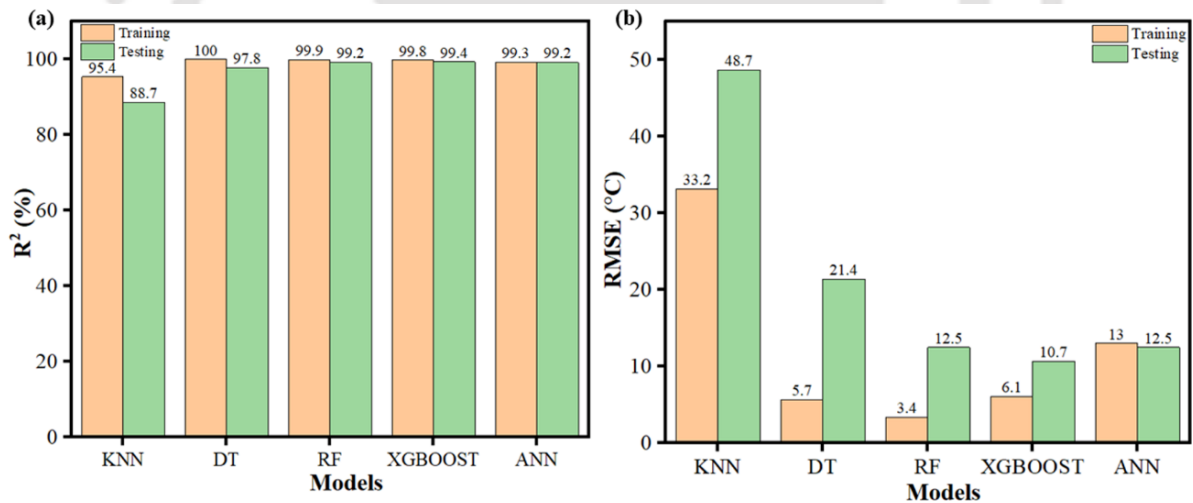


Figure 5.3: Evaluation metrics utilized for different models: (a) R² score, (b) RMSE of both training and testing datasets for an arc power ranging from 1.28 kW to 3.16 kW and deposition speed of 3.3 to 15 mm/s

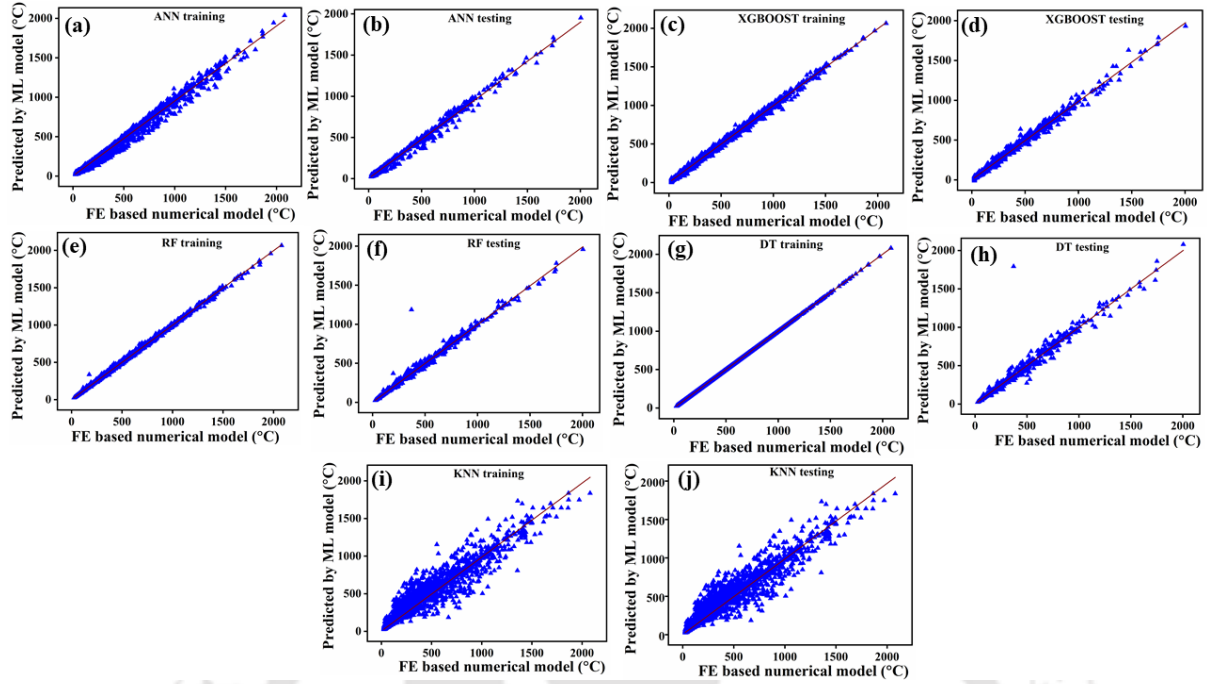


Figure 5.4: Comparison of the predicted temperature ML models and FE-based numerical model on training and testing datasets for an arc power ranging from 1.28 kW to 3.16 kW and deposition speed of 3.3 to 15 mm/s.

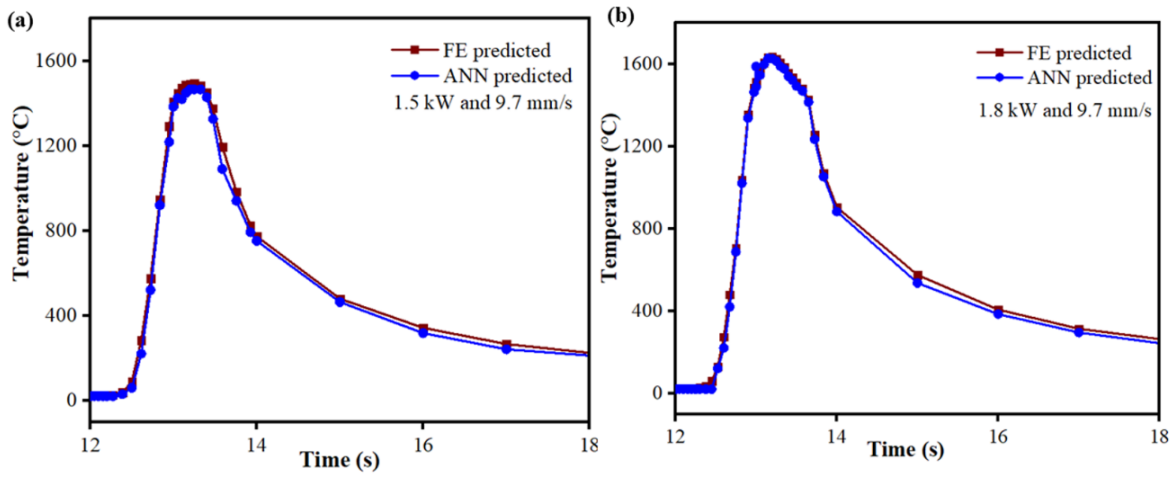


Figure 5.5: Transient temperature distribution prediction by digital twin model at different deposition variants.

5.2.3 Bidirectional prediction of maximum temperature

ML models with the highest accuracy are utilized for both forward and inverse prediction between the deposition attributes and peak temperature. To evaluate the maximum temperature for a deposition attribute the models (ANN, DT, RF, and XGBOOST) are considered and hyper-tuned to get better accuracy. Table 5.2 indicates the comparison between FE and ML predicted maximum temperature by all four models. The predicted peak temperature is closer to the FE values with an error of less than 10%. For the prediction of deposition attributes pertaining to the targeted peak temperature, both ANN and XGBOOST models are used. First, the velocity and temperature are considered as features and power is predicted. Further, power and temperature are utilized as input and velocity as a output. On these two independent datasets, ANN model performs quite well ($R^2 = 0.99$ for power and velocity) as compared to XGBOOST ($R^2 = 0.95$ for power and $R^2 = 0.85$) (Figure 5.6). Table 3 depicts the output of inverse prediction of power and velocity and their close resemblance with actual values.

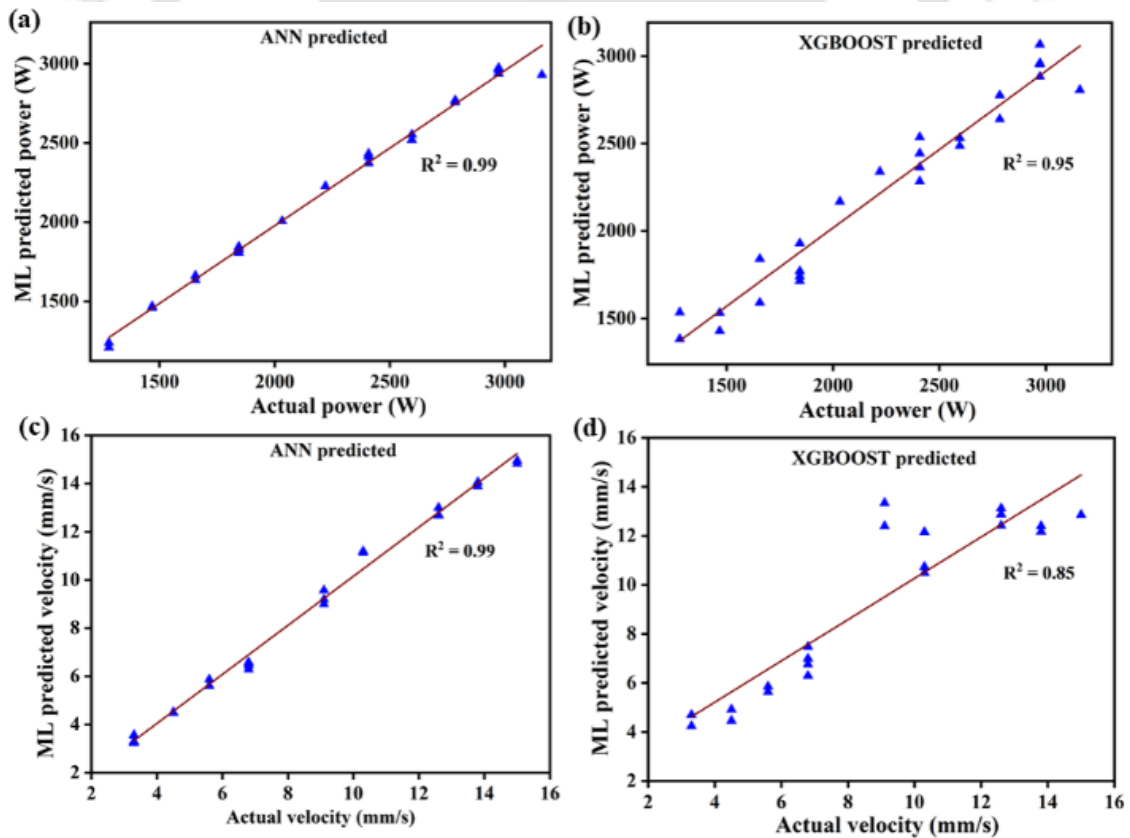


Figure 5.6: Comparison of the ml predicted power and velocity with actual values considered for numerical simulation for the peak temperature datasets.

Table 5.2: Prediction of the peak temperature on validation deposition attributes with an error by ML model.

Sl. No.	Model	Power (kW)	Velocity (mm/s)	FE predicted (°C)	ML predicted (°C)	Error (%)
1	ANN	1.5	9.7	1481	1386.5	6.4
2	ANN	1.65	9.7	1620	1557	3.8
3	ANN	1.8	9.7	1725	1673.8	2.9
4	DT	1.5	9.7	1481	1387.6	6.3
5	DT	1.65	9.7	1620	1496	7.6
6	DT	1.8	9.7	1725	1583	8.2
7	RF	1.5	9.7	1481	1398.4	5.5
8	RF	1.65	9.7	1620	1570.9	3
9	RF	1.8	9.7	1725	1669	3.2
10	XGBOOST	1.5	9.7	1481	1397.4	5.6
11	XGBOOST	1.65	9.7	1620	1581.9	2.3
12	XGBOOST	1.8	9.7	1720	1645.8	4.3

Table 5.3: Comparison of the actual and predicted power by the ANN and XGBOOST models.

Sl. No	Model	Peak Temperature (°C)	Actual Velocity (mm/s)	Predicted Velocity (mm/s)	Error (%)	Actual Power (W)	Predicted Power (W)	Error (%)
1	ANN	2566	3.3	3.2	3	2972	2972.1	0.003
2	ANN	2784	5.6	5.6	0	2784	2770.0	0.5
3	ANN	2074	6.8	6.5	4.4	2972	2974.2	0.07

4	ANN	1786	4.5	4.5	0	2032	2007.3	1.2
5	ANN	1783	10.3	11.1	7.7	2972	2937.6	1.1
6	XGBOOST	2566	3.3	4.2	27	2972	3066.1	3.1
7	XGBOOST	2085	5.6	5.8	3.5	2784	2776.9	0.25
8	XGBOOST	2074	6.8	7.0	2.9	2972	2952.9	0.64
9	XGBOOST	1786	4.5	4.9	8.8	2032	2169.1	6.7
10	XGBOOST	1783	10.3	10.7	3.8	2972	2882.2	3

The correlation between the process parameters is represented by Pearson's correlation matrix. For the transient temperature profile, enhancement of continuing deposition value of temperature is analogous to the practical scenario of fabricating a component by the WAAM process. On increasing arc power, the maximum temperature increases, while on increasing velocity, it is negatively correlated (-0.55). It indicates that the generated datasets from a well-tested FE-model is correlated with the physics of the process behind the deposition process. Hence an efficient PIML model can be developed for any deposition attributes in AM industry.

5.2.4 Experimental validation of residual stress

Figure 5.7 depicts a comparison between the numerically predicted and experimentally measured residual stresses, highlighting both longitudinal (S_{11}) and transverse (S_{22}) components obtained using a portable XRD system. The simulation results closely align with the experimental data, validating the reliability of the numerical approach in capturing the residual stress distribution. Notably, the S_{11} exhibits significantly higher magnitudes than the S_{22} , with a clear distinction between tensile and compressive regions. This pronounced anisotropy arises from the directional nature of heat input in additive manufacturing processes. During layer-by-layer deposition, intense localized heating along the deposition path induces steep thermal gradients in the longitudinal direction, resulting in substantial tensile stresses near the surface and compressive stresses in the sub-surface or heat-affected zones. In contrast, the transverse direction is subjected to comparatively uniform thermal exposure, leading to smaller thermal strains and correspondingly lower residual stress magnitudes.

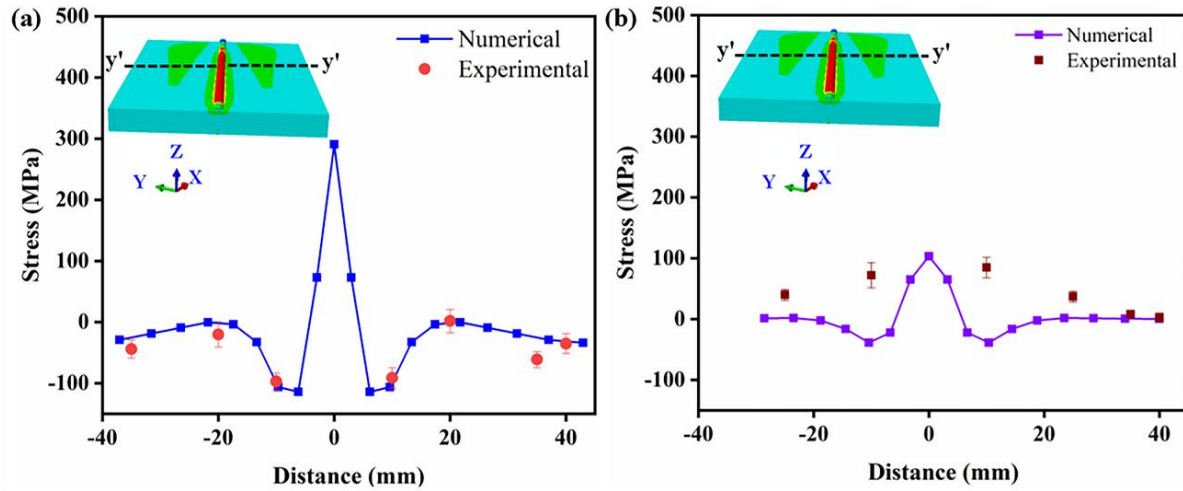


Figure 5.7: Validation of physics-based numerical model with experimental results: (a) longitudinal residual stress; and (b) transverse residual stress at deposition attribute of 2.6 kW and 8 mm/s.

5.2.5 Prediction of the transient residual stress profiles

Figure 5.8 depicts a progressive improvement in model performance reflecting the increasing ability of LSTM, BiLSTM, GRU and TCN architecture, respectively, to capture the complex temporal dynamics of residual stress evolution. LSTM, with its unidirectional memory flow, struggles to fully retain long-range dependencies, resulting in lower accuracy ($R^2 = 0.72$, RMSE = 96.8 MPa) (Figure 5.8 a). BiLSTM enhances learning by accessing both past and future time steps, leading to better stress pattern recognition ($R^2 = 0.85$, RMSE = 67.6 MPa) (Figure 5.8b). GRU further refines temporal modeling through a simplified yet effective gating mechanism, allowing for more efficient learning of stress transitions ($R^2 = 0.97$, RMSE = 12.5 MPa) (Figure 5.8c). TCN surpasses all by leveraging dilated convolutions, which capture long-range dependencies without sequential bottlenecks, enabling precise modeling of multiscale stress fluctuations ($R^2 = 0.99$, RMSE = 4.7 MPa) (Figure 5.8d). This clearly establishes TCN as the most capable architecture for learning the physics-informed temporal behavior of residual stress in DED process.

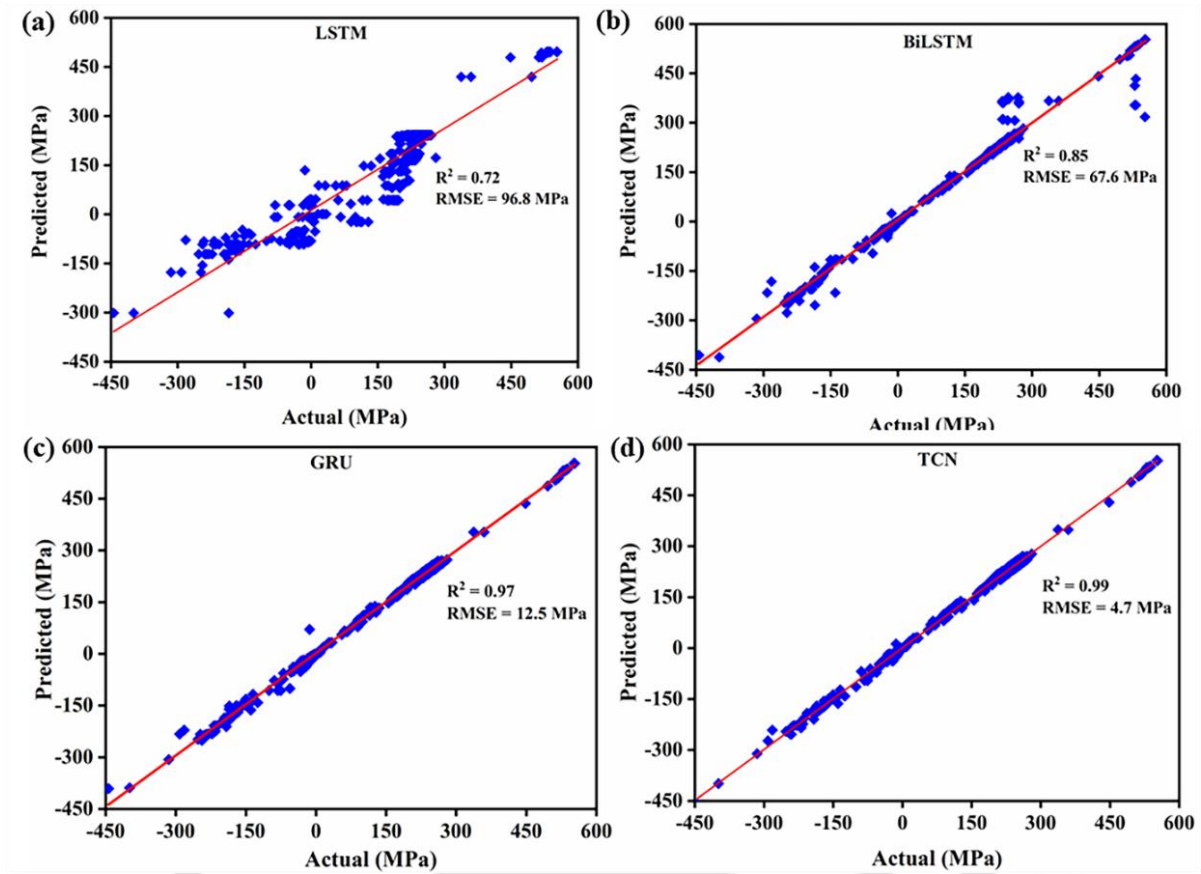


Figure 5.8: Comparison of predicted residual stress with numerically computed testing datasets varying from 85 J/mm to 950 J/mm.

Comparative analysis of predicted stress profiles over the full thermal cycle, highlighting distinct differences in how each deep learning model captures the transient nature of residual stress evolution (Figure 5.9). From the onset of deposition ($t = 2.00$ s) to the end of cooling, LSTM, BiLSTM, and GRU exhibit noticeable lag in predicting the actual stress curve. The LSTM model captures the initial compressive-to-tensile transition but fails to represent sharp tensile fluctuations during cooling, resulting in a smoothed profile with poor alignment ($R^2 = 0.74$, $RMSE = 115.6$ MPa; Figure 5.9a). BiLSTM improves trend recognition through bidirectional context but struggles with abrupt stress inflections from thermal gradients ($R^2 = 0.82$, $RMSE = 74.5$ MPa; Figure 5.9b). GRU, aided by efficient gating, better captures long-range dependencies but shows phase lag at the cooling onset and misses finer oscillations ($R^2 = 0.95$, $RMSE = 37.5$ MPa; Figure 5.9c). In contrast, TCN accurately reconstructs the full non-linear stress profile from start to finish, effectively modeling rapid fluctuations and long-term

trends via dilated convolutions. Its prediction closely matches the actual stress evolution, achieving near-perfect accuracy ($R^2 = 0.99$, RMSE = 6.4 MPa; Figure 5.10d).

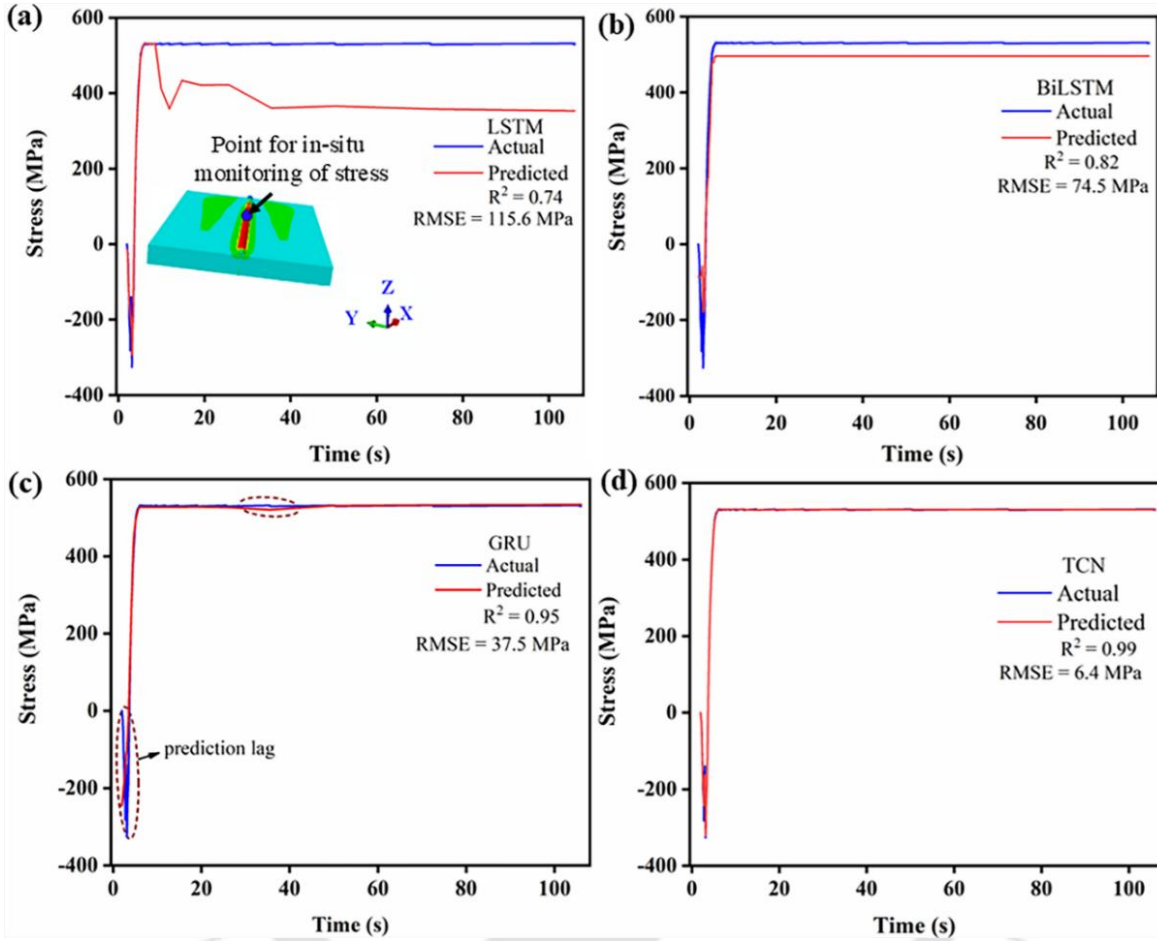


Figure 5.9: Prediction of residual stress evolution by RNN based models: (a) LSTM (b) BiLSTM, (c) GRU, and (d) TCN.

5.3 AI driven thermo-mechanical analysis of multi-layer deposits

Inter-layer dwell time (D_{TM}) is a key attribute for controlling thermo-mechanical behavior in multi-layer deposition by wire-based DED process as it governs reheating, cooling rates, and the phase transformation kinetics that set residual stress magnitudes and spatial gradients. yet direct in-situ characterization is cumbersome and high-fidelity finite-element simulation across wide dwell-time ranges is computationally expensive, which limits rapid process exploration and on-the-fly optimization. To bridge this gap, we couple an experimentally validated FE framework with physics-informed deep learning (PIDL) so that time-resolved

thermal and stress trajectories generated. Under known conditions become a training corpus for surrogate models that preserve physical trends while achieving orders-of-magnitude speedups. Within this AI-assisted, D_{TM} is treated as a key input alongside process parameters, enabling accurate prediction of nonlinear transient temperature fields and residual stress paths, credible interpolation within the validated domain, and cautious extrapolation to nearby dwell-time regimes. Rigorous comparison against experimental observations establishes fidelity, after which the same models support inverse use cases in which target responses such as reduced tensile stress are specified and feasible D_{TM} values are inferred subject to process constraints. The result is a computationally efficient and physically grounded route for designing thin wall builds where D_{TM} is optimized to mitigate tensile residual stress and stabilize microstructure.

5.3.1 Effect of inter-layer dwell time on residual stress generation

Figure 5.10 illustrates the temperature history in single-track, multi-layer deposition of ferritic steel for inter-layer dwell time of 100 s. Figure 5.10a depicts that the thermocouples are attached to both the substrate and deposited materials (after the deposition of five layers). The calculated temperature profiles are in good agreement with the experimental results (Figure 5.10 b, c). It is noteworthy that the maximum temperature in each thermal cycle keeps on decreasing, which is attributed to a continuous increase in the height of the wall. The peak temperature (thermocouple point) in the deposited sample is higher in magnitude ($\sim 1006.2^\circ\text{C}$) as compared to the substrate ($\sim 350^\circ\text{C}$). The volume of the substrate material is larger (the volumetric ratio between the substrate and deposit is 11); hence, it acts as a heat sink for the deposited layer. However, the heat transfer area for printed walls is less and the thermocouple is attached closer to the molten pool. All these factors make wide difference in peak temperature of substrate and printed thin wall. The heat source parameters are calibrated using a single bead model. Figure 5.10d indicates a molten pool that closely matches experimental data obtained at a deposition power of 2.8 kW and a speed of 12.6 mm/s. Both the numerically computed and experimentally obtained free surface profile of the deposited material is parabolic in nature. Regions with grey color depict the molten pool temperature, while the mushy zone of the material (difference in solidus and liquidus temperature $\sim 80^\circ\text{C}$) is shown in red color.

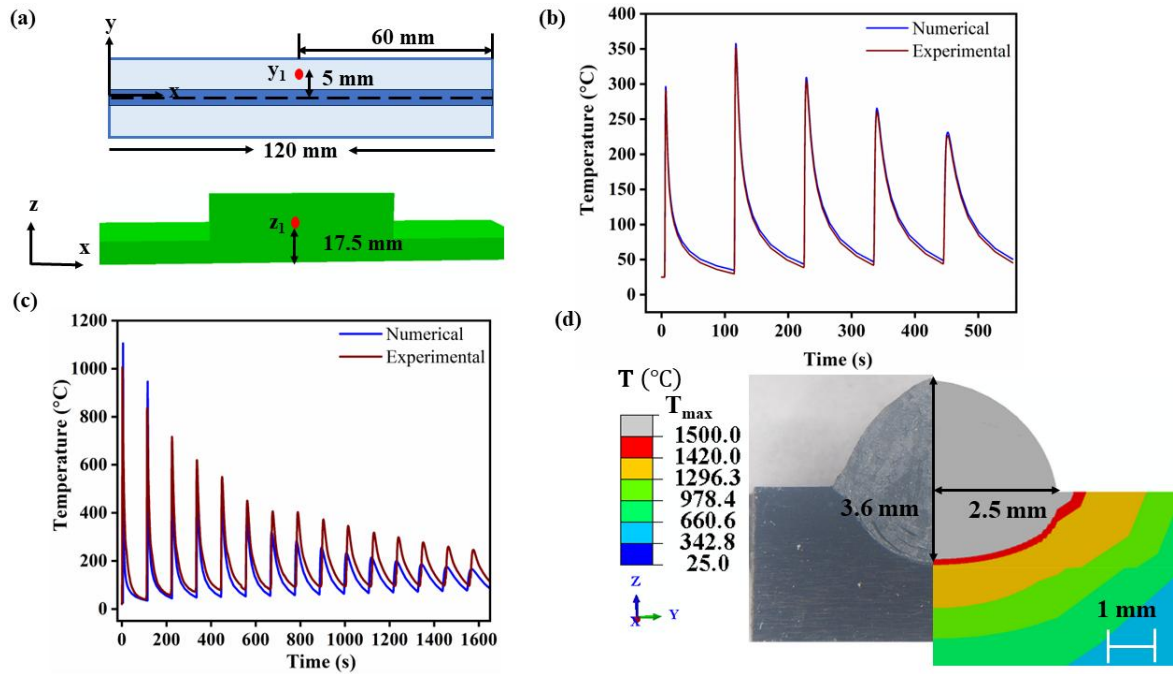


Figure 5.10: Comparison of the temperature profiles at inter-layer dwell time of 100 s: (a) location of thermocouple points; (b) temperature history of substrate at location y_1 ; (c) thermal cycles of first fifteen layers at location z_1 ; (d) comparison of bead profile.

Figure 5.11 represents the spatial temperature distribution at the middle of the 5th, 10th, and 20th layers for the inter-layer dwell times of 100 s and 400 s, respectively. In the middle of the deposition, the molten pool is compressed, and it is elongated behind the arc (Figure 5.11(a-f)). However, the size of the mushy zone is found to vary at trailing (wider) and leading (thinner) edges. On depositing the stack of layers from 5th to 20th, the temperature is continuously increased from 2375°C to 2530°C (for 100 s), and 1941°C to 2050°C for 400 s dwell-time. The heat loss is much more for low dwell-time because of high temperature differences. On increasing the dwell time from 100 s to 400 s, the peak temperature differences are almost of similar order (434.7 °C, 447.4°C, and 479.9°C for 5th, 10th, and 20th layers) that indicates the heat dissipation rate is almost constant.

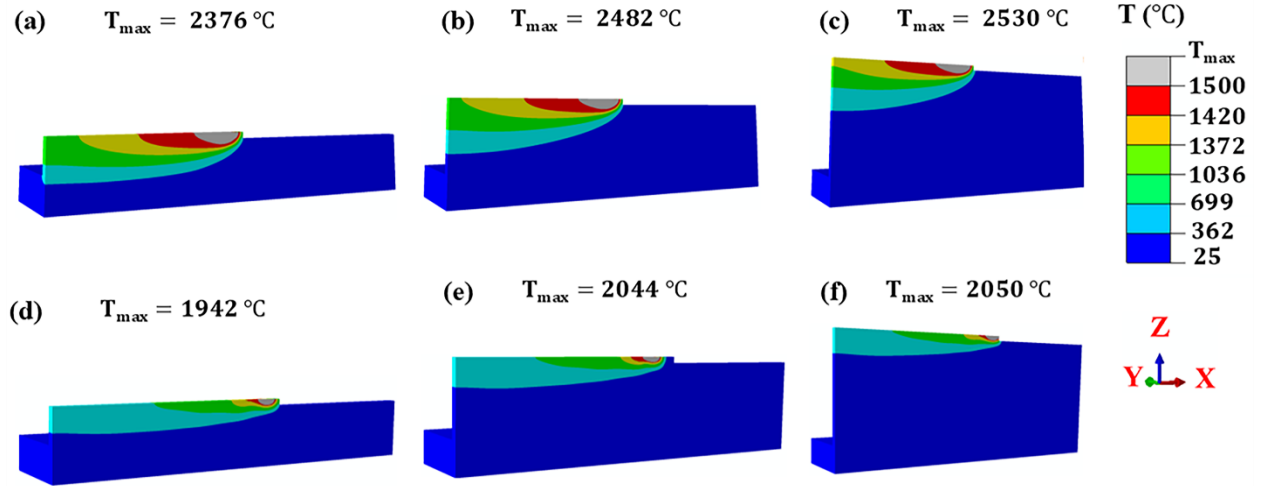


Figure 5.11: Spatial variation of temperature along the build direction at the middle of the deposition of the 5th layer, 10th layer, and 20th layer for 100 s (a, b, c), and 400 s (d, e, f) inter-layer dwell times.

Figure 5.12 depicts the evolution of temperature and longitudinal residual stress (S_{11}) at two different dwell phases. The counting of temperature is considered at the end of the deposition of the 5th layer and cooling phase is defined till the completion of dwell-time. Figure 5.12a indicates that the temperature gradient becomes almost flat within 25 s and afterward the uniform temperature decrement is very low. The maximum temperature difference of 588 °C is achieved after 100 s dwell time. However, similar trend is observed for 400 s dwell-time where the maximum temperature difference is achieved as 660.2 °C (Figure 5.12b). These particular temperature distributions influence the residual stress (longitudinal) distribution. At the initial phase of the dwell-time, the liquid material starts cooling that is characterized by low and non-uniform distribution of stress. At the end of dwell-phase, the spatial gradient of temperature is almost zero. It is accustomed to a uniform pattern of residual stress settlement of higher magnitude (Figure 5.12c). Similar analogy is also applicable for 400 s dwell-time. On increasing the dwell time, the temperature difference keeps on increasing ($\sim 72.2^\circ\text{C}$) as well the residual stress (230.6 to 282.7 MPa). However, the gradient of temperature increment is more than longitudinal residual stress. Overall, tensile residual stress is developed along the deposited length after 5th layer of deposition. Here, the bulk material expansion and contraction

between the layers induces tensile residual stress. However, the deposited materials are free from any restraint at the extreme edges, which induces almost zero residual stress.

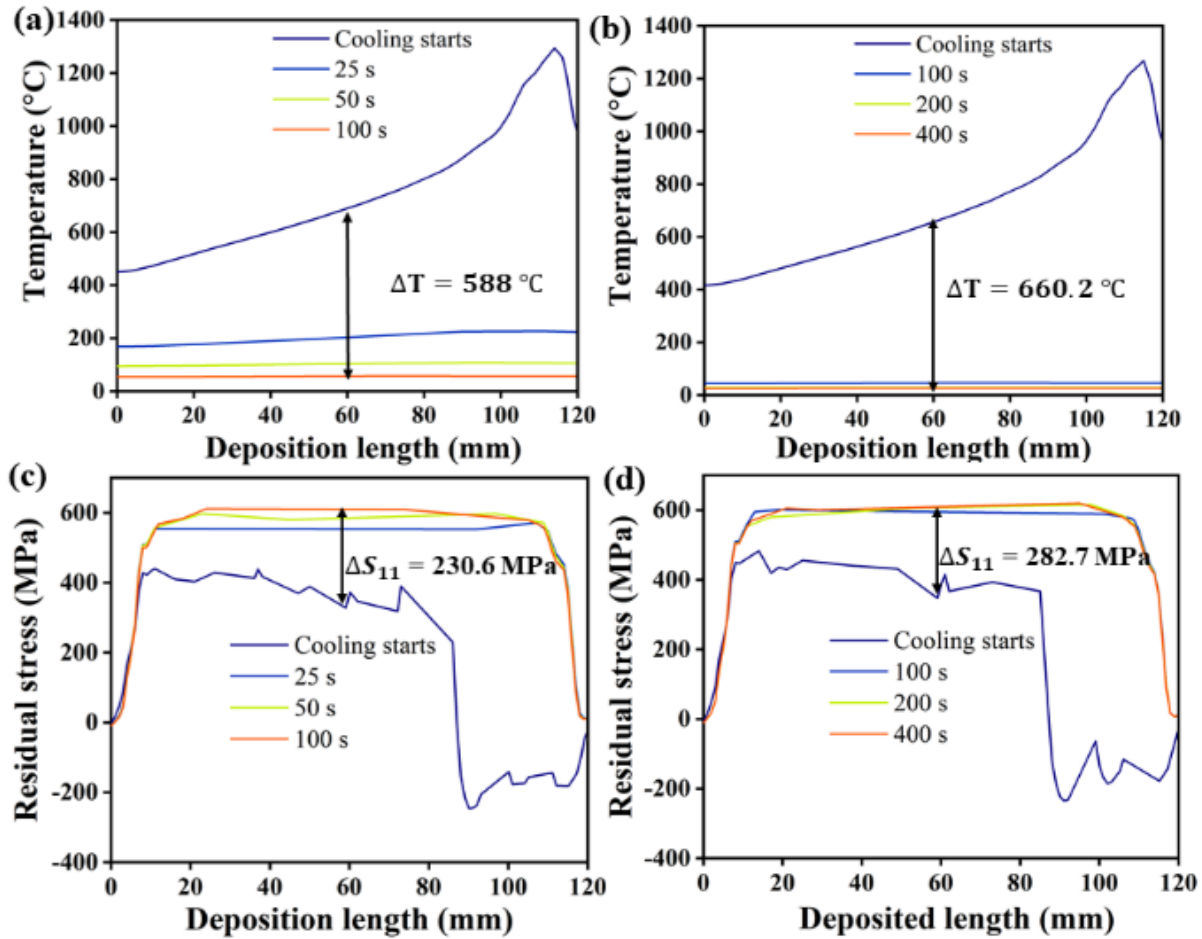


Figure 5.12: Evolution of temperature and residual stress at the end of 5th layer deposition for inter-layer dwell times of (a, c) 100 s and (b d) 400 s along the deposition length.

The distribution of three components of residual stress, S_{11} (longitudinal), S_{22} (transverse), and S_{33} (through-thickness) for 400 s dwell-time is depicted in Figure 5.13. The nature of these stresses is changed from compressive to tensile at the interface of the deposits and substrate. Out of all these, tensile stresses in the longitudinal direction are higher in magnitude as compared to the other two along the build direction of the fabricated thin wall (Figure 5.13 a). This occurs due to the shrinkage of the molten metal at the end of deposited layer without much constraint from top layers and no compensation of the shrinkage volume during solidification. A higher magnitude of this stress significantly affects the mechanical properties of the

component, especially the fatigue strength. It increases susceptibility to delamination and warping exceeding the yield strength. Hence, the variation of this stress is considered for further analysis as it is critical among all. However, the compressive residual stress (S_{11}) is observed in very localized position near the free end of almost each layer. Similarly, the transverse compressive residual stress (S_{22}) is observed in the localized position of each layer. The through-thickness compressive residual stress (S_{33}) zone is much more than S_{11} and S_{22} . Even the higher magnitude of longitudinal tensile residual stress zone is much more expanded than transverse and through-thickness residual stress.

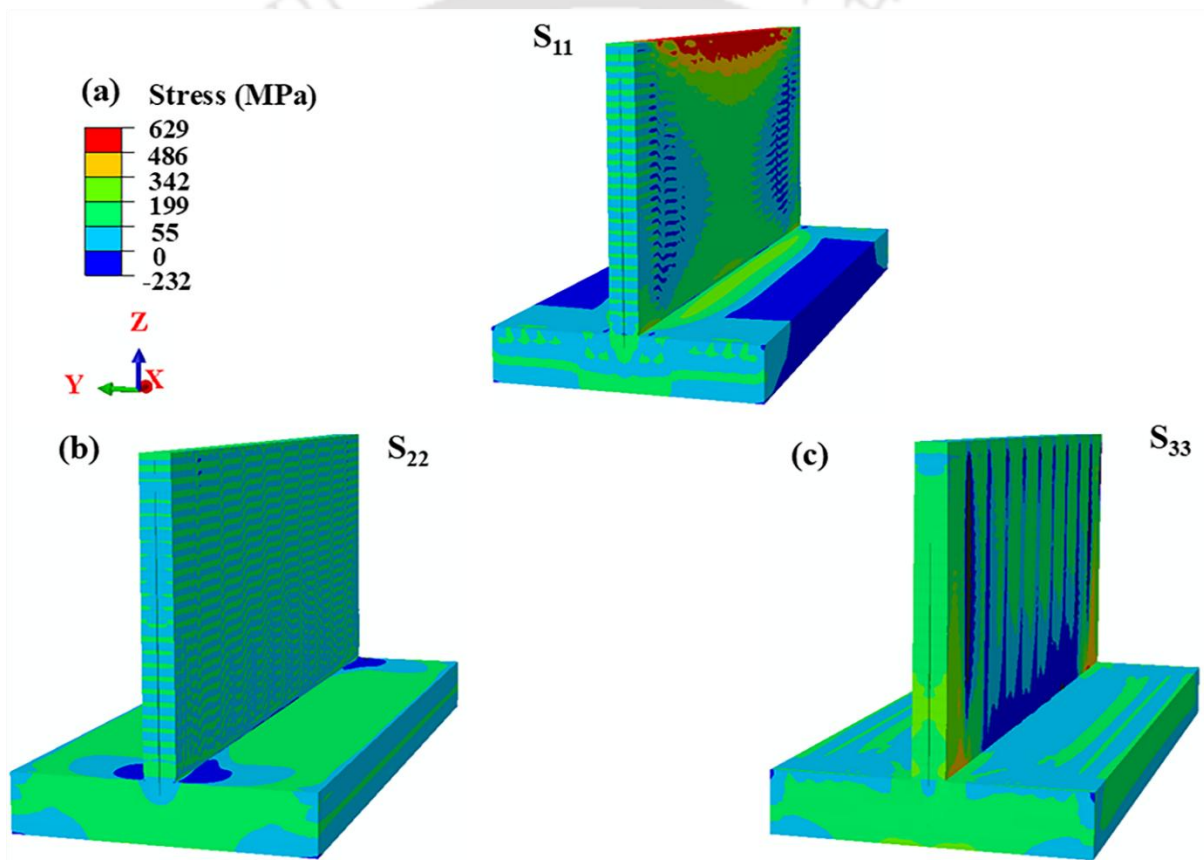


Figure 5.13: Elucidation of the different components of the residual stress on the completion of inter-layer dwell time of 400 s between the stack of deposited layers along (a) x-direction (S_{11}); (b) y-direction (S_{22}); and (c) z-direction (S_{33}).

The longitudinal residual stress (S_{11}) is measured along the deposition direction ($x' - x'$) and build direction ($z' - z'$). The comparison of numerically calculated and experimentally

evaluated residual stresses at two dwell-times (100 s and 400 s) is depicted in Figure 5.14. The measurements of the stresses using portable XRD are repeated three times at a point, and mean values are reported. Similar trends of the profile between the numerically computed and recorded values are observed. A small difference between the simulated and measured values is justifiable. The ignorance of the phase transformation effect has a significant impact on the development of the residual stress [169]. The present model does not account the phase transformation strain and hence the small discrepancy is observed. Figure 5.14 (a and b) indicates the high magnitude of tensile stress at the middle of the deposit (~ 600 MPa for 100 s dwell time and ~ 650 MPa for 400 s dwell time). Figure 5.14 (c and d) indicates a significant enhancement in stress from the substrate to the top of the deposit along the build direction. On increasing dwell time, stress induced in the component is higher in magnitude in both deposition and build direction. At lower dwell-time, the preheating effect is pronounced, and hence low temperature gradient exists than a high value of dwell-time.

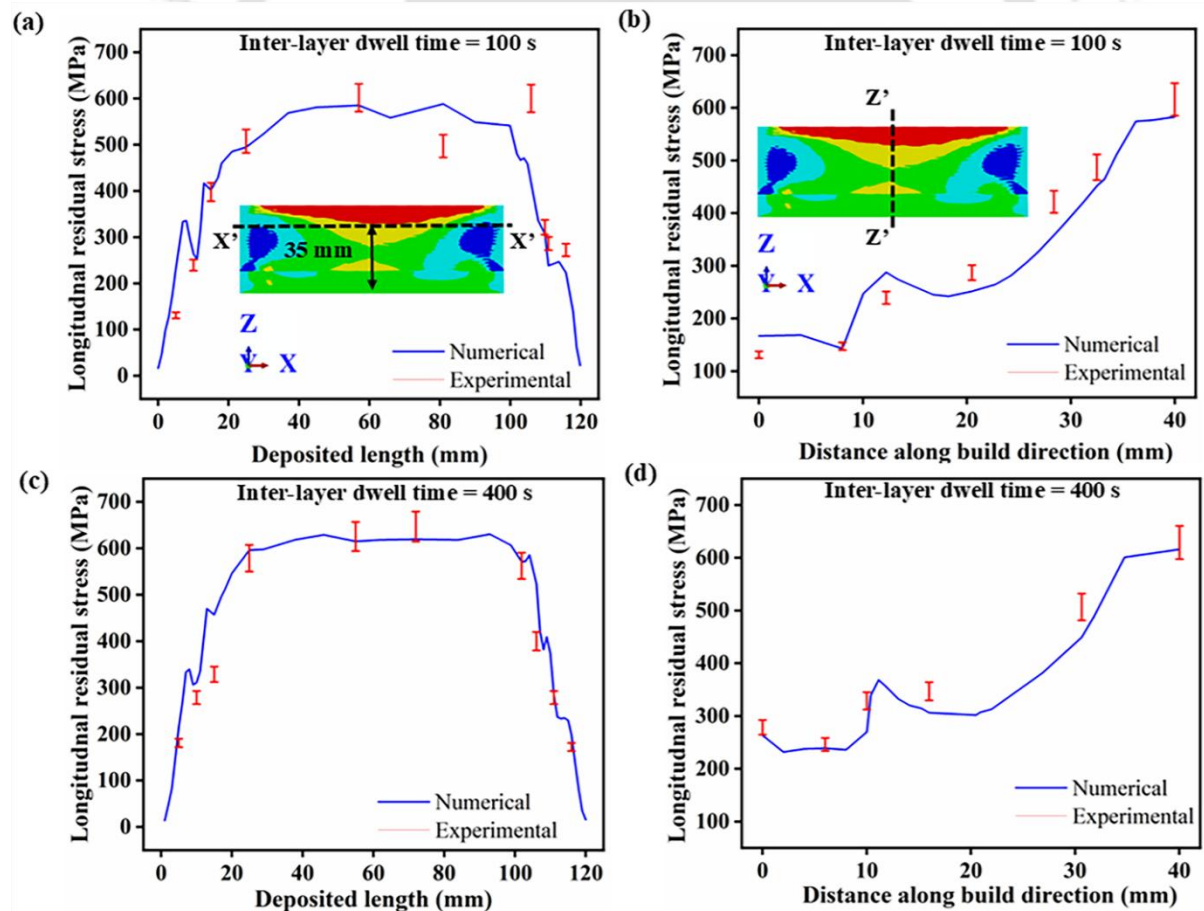


Figure 5.14: Validation of longitudinal residual stress (S_{11}) along the deposition and build direction on enhancing the inter-layer dwell time from 100 s (a, b) to 400 s (c, d).

The spatial variation of the longitudinal stress (S_{11}) at the end of the cooling steps of the 5th, 10th, and 20th layers for 100 s and 400 s are interplayed in Figure 5.15. In all the deposits, the maximum tensile stress is present at the top of the deposits (red and yellow contour). On further depositing the layers, the tensile residual stress is reduced (644 MPa to 610 MPa for 100 s, 651 MPa to 620 MPa for 400 s). The reheating and re-solidification of the deposits equilibrate the tensile stress and effectively reduce the maximum magnitude. However, a significant enhancement in the difference of stress is noted in triggering the dwell times (7 MPa for the 5th layer, 15 MPa for the 10th layer, and 35 MPa for the 20th layer). The compressive residual stress is induced up to the mid-height of the fabricated wall at the start and the end (Figure 5.15 c and f). Overall, the maximum magnitude of compressive residual stress gradually reduces with the increasing number of layers.

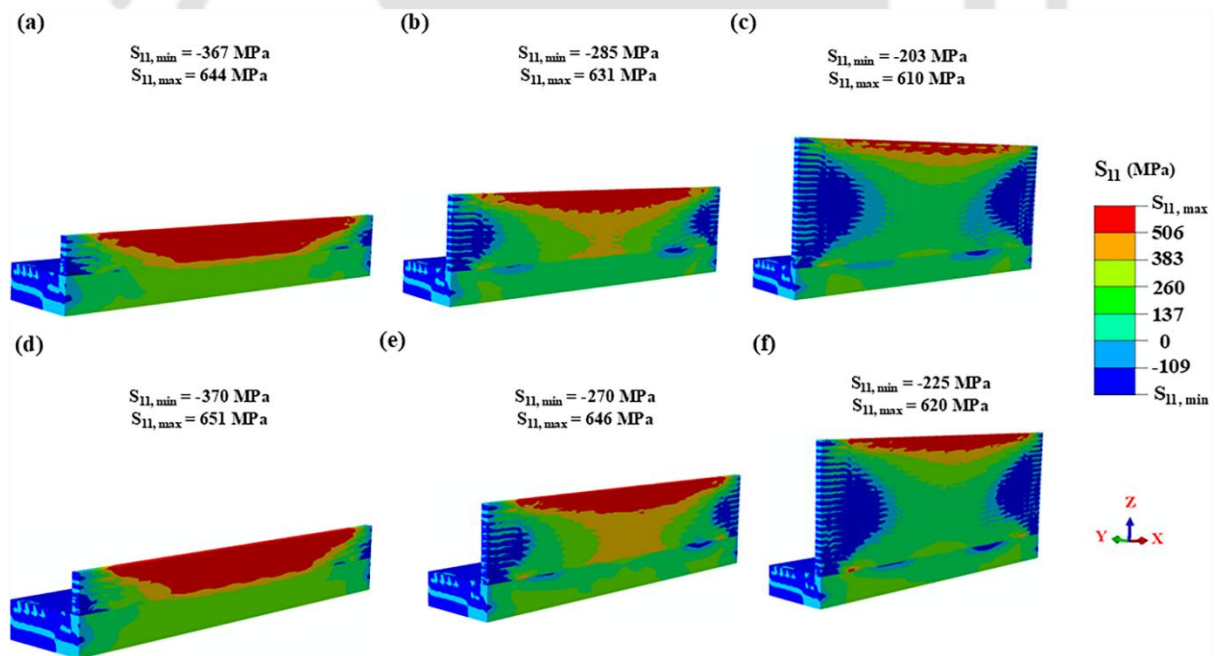


Figure 5.15: Distribution of residual stress (S_{11}) along the longitudinal direction at the end of the deposition of the 5th layer, 10th layer, and 20th layer for 100 s (a, b, c), and 400 s (d, e, f) inter-layer dwell time.

5.3.2 Forward prediction by PIDL model

The interlinking between the dwell times and the temporal and spatial variations of the temperature and residual stress is the primary objective of the present work. Hence, adequate datasets are augmented from a physics-based numerical model by performing the numerical simulation as a function of dwell-times. The range of dwell times is considered within the experimental value (100 s and 400 s) to train the more realistic data driven PIDL model. Figure 5.16 shows the distribution of temperature and residual stresses at each node along the build direction. Along the build direction, the maximum inter-pass temperature drastically reduces (413.4 °C to 25.9 °C) for dwell-time 100 s to 400 s. However, the maximum inter-pass residual stress increases from 95.3 MPa to 634.8 MPa on increasing the dwell times from 100 s to 400 s. Here, the discrete data are collected from the distribution of temperature and residual stress profiles rather than only selective data points. The pattern of temperature and residual stress profiles are evaluated using Pearson's correlation matrix where the scores vary from -1 to 1. A positive correlation of stress with dwell time (0.3) and height (0.74) and negative with temperature (-0.14) are established here. Here, the datasets are created by imparting the physics of the process through an experimentally validated numerical process model.

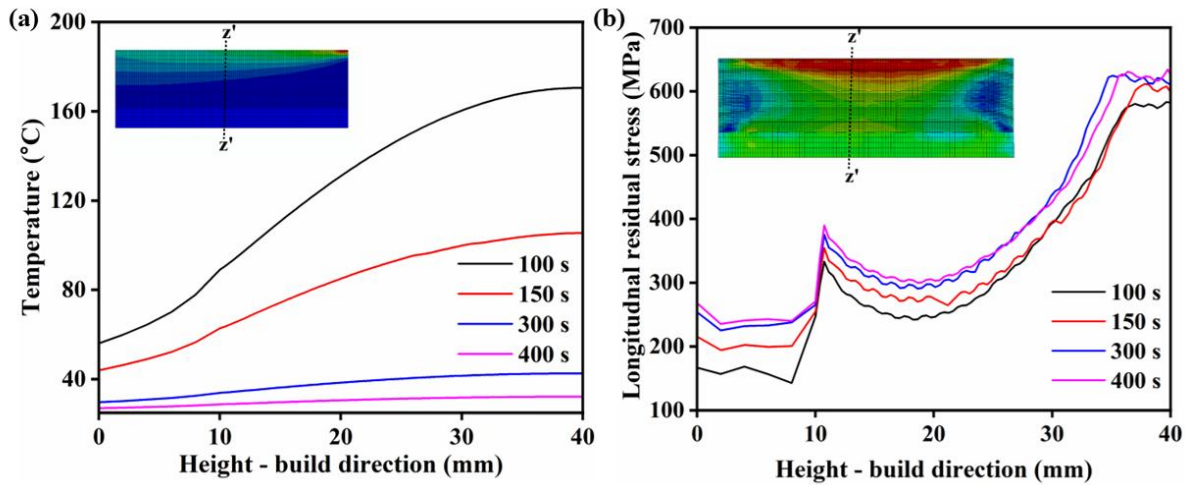


Figure 5.16: Effect of inter-layer dwell time along build direction on (a) temperature at the end of the deposition process; (b) residual stress distribution at the end of the inter-layer dwell time.

The performance of the PIDL models is significantly altered by the number of hidden layers for the same training and testing sets of data. All these architectures of neural network are accomplished using 90% of the data for training and the remaining for validation. The RMSE value reduces from 13.8 °C to 1.1 °C on training and 15.2 °C to 1.1 °C on testing. However, the accuracy of the PIDL model is enhanced from 96% to 99.9% on training and 95.2% to 99.9% on testing for temperature data. For stress analysis, the accuracy of the model increases from 63.9% to 99.7% on training and 61.7% to 99.5% on testing. Considering the highest prediction accuracy (~99.9%) and the lowest prediction error, the optimal PIDL model is Model 5. While fitting the dataset with DL models, loss between actual and predicted values is reduced continuously with an increase in the number of epochs by adjusting the initially randomized weight and bias (backpropagation technique) as depicted in Figure 5.17. Ideally, the loss should approach zero in each epoch. It is obvious that the RMSE value for temperature reduces from 133.8 °C to 0.7 °C up to 2,500 epochs, and further it becomes flat. For the stress analysis, it reduces from 397.7 MPa to 10.3 MPa up to 4000 epochs, and later it becomes flat. One can see that the difference in evaluated profiles on validation sets is insignificant which depicts that the optimized PIDL model is free from variance problems for both temperature and residual stress analysis.

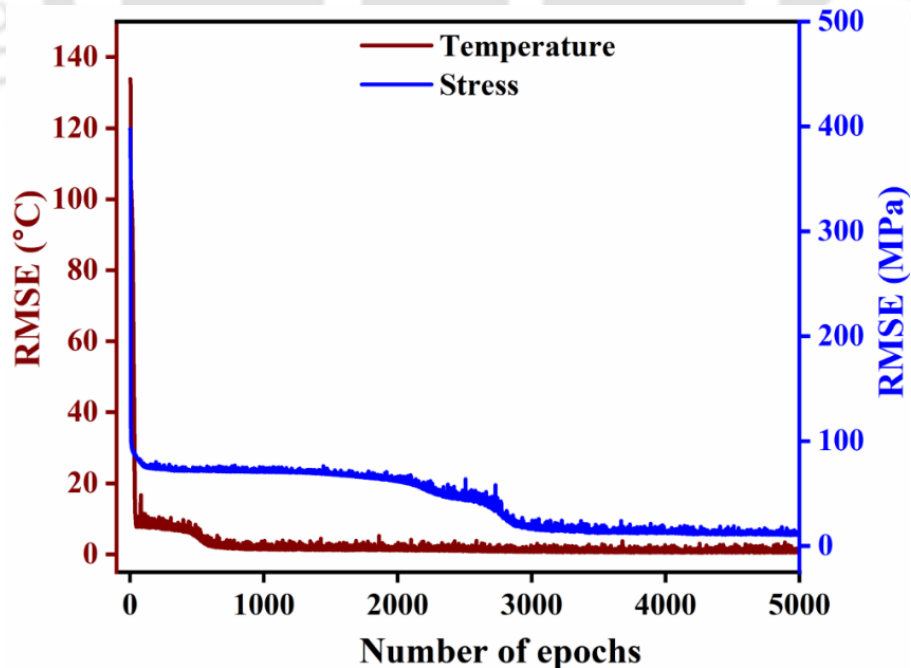


Figure 5.17: Computed loss of PIDL Model-5 with varying number of epochs on validation datasets of temperature and stress for inter-layer dwell time range of 100 s to 400 s.

Four more experiments are performed to fabricate thin wall components at interpolated and extrapolated inter-layer dwell times that are not included in training of the PIDL model. The purpose is to test the proficiency of the developed PIDL model at these unknown dwell-times. Figure 5.18 depicts the endorsement of the PIDL model to predict temperature and residual stresses on the interpolation cases. Total deposition height of the printed thin wall structure is 40 mm, each layer thickness is 2 mm. The temperature profile is recorded at a fixed location on the completion of the 20 layers including the inter-layer dwell time. The residual stress is also measured using portable XRD at different points along the build direction. The close resemblance of the predicted non-linear thermal and residual stress profiles is clearly observed by the robustness of the developed PIDL model.

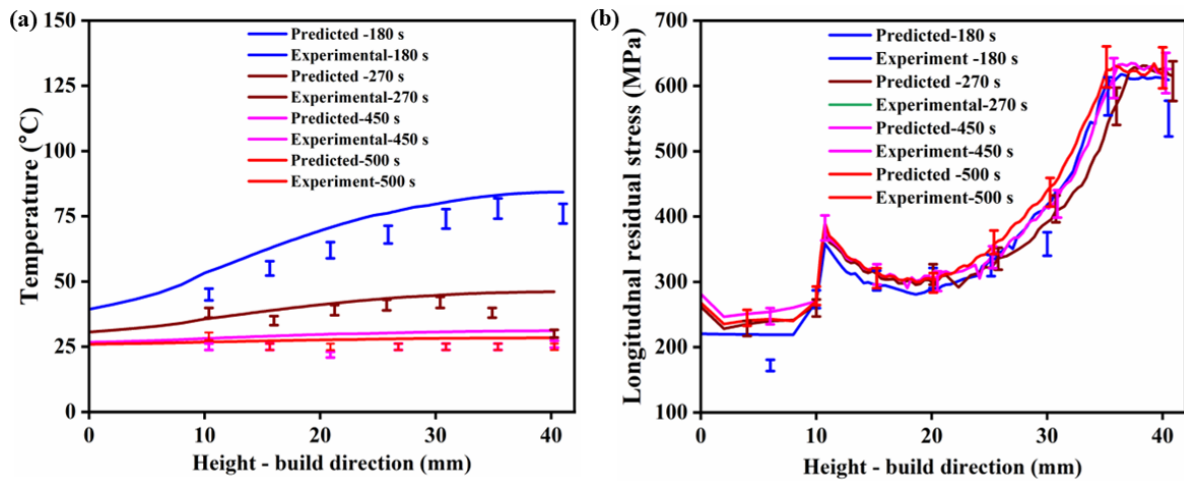


Figure 5.18: Comparison of the temperature and residual stress profiles between the PIDL model and experimental results along the build direction: (a) depicts temperature validation, while (b) represents stress validation for both interpolated (180 s, 270 s) and extrapolated (450 s, 500 s) cases.

On similar interpolation and extrapolation data sets, additional simulations are also carried out as testing attributes of the PIDL model. Figure 5.19 demonstrates the effectiveness of PIDL model for predicting temperature and residual stress at interpolated dwell-times. A close match

between the predicted and actual non-linear thermal and residual stress profiles are obvious. As dwell time increases from 180 s to 270 s, the maximum inter-pass temperature reduces from 86°C to 47°C, while the inter-pass residual stresses increase from 618 MPa to 630 MPa. For the interpolation case, only minor discrepancies are observed in the predicted non-linear profiles (Figure 5.20 a and b). It is obvious that the model correctly captures the physics of DED process from the datasets. On extrapolated cases (450 s and 500 s), the predicted inter-pass temperatures between the layers by PIDL model tending towards the ambient condition of deposited material up to 10 mm height of first five layers (Figures 5.19 c and d). With the increase of stack of layers, the inter-pass temperature ended to 30°C. At dwell time of 500 s, there is a slight deviation between the predicted and numerically computed residual stress profiles (Figure 5.19 d). Overall, the predicted results by PIDL model indicate the effectiveness in capturing the heat transfer phenomena during cooling period that have significant impact on evolution of residual stress at test cases outside the training range.

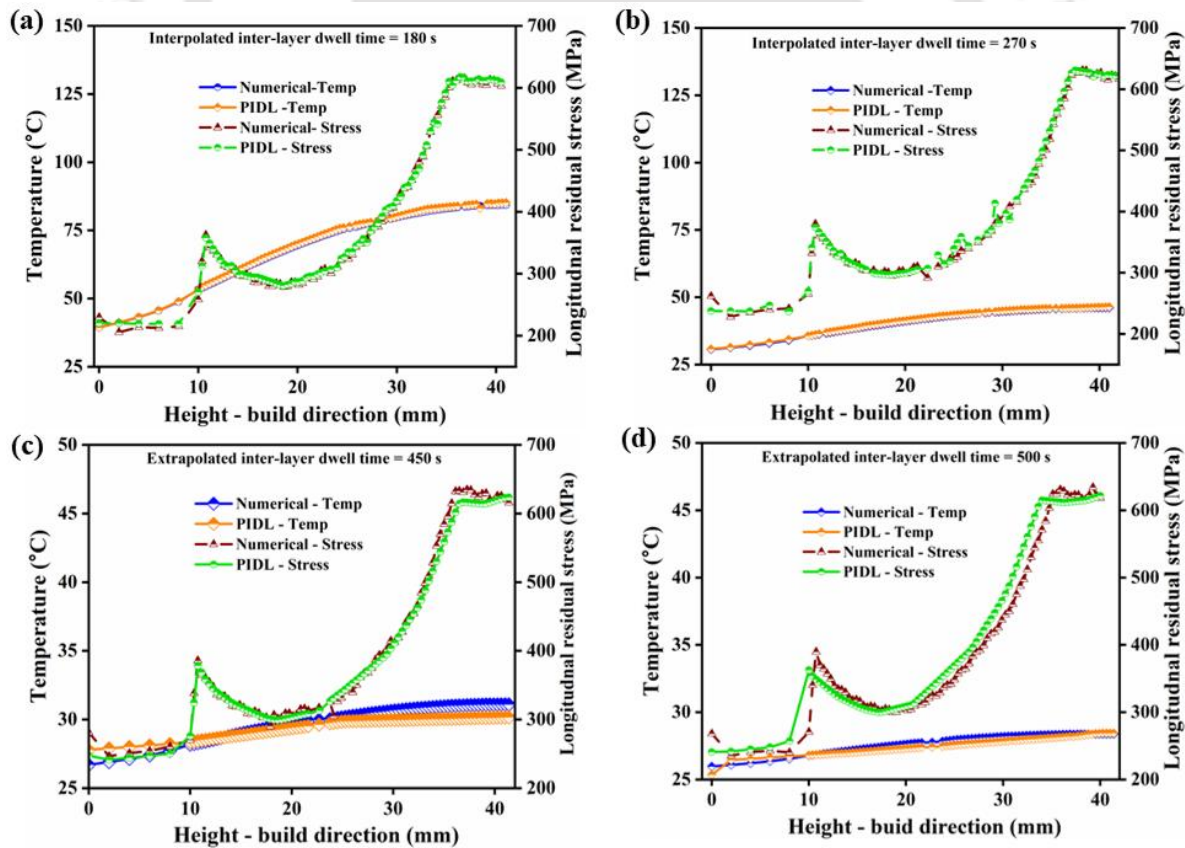


Figure 5.19: Comparison of temperature and residual stress profiles between PIDL model and numerical model along the build direction: (a, b) interpolated inter-layer dwell times of 180 seconds and 270 seconds, and (c, d) extrapolated inter-layer dwell times of 450 seconds and 500 seconds.

Table 5.4 presents the MAE by PIDL Model 5 for an experimentally measured residual stress (σ_{RS}) value at discrete points of thin wall. The performance of the model reveals important insights into its predictive capabilities in both interpolated and extrapolated scenarios. At 180 s and 270 s dwell-times, the PIDL model demonstrates high accuracy, with MAE values ranging from 1.5% to 3.5%, indicating a strong alignment between the predicted and actual residual stress values. For example, at a build height of 10 mm, the MAE is just 3% at 180 s and decreases to 1.5% at 270 s, showing that the model's predictions closely match the experimental results within this range. Similarly, at a build height of 40 mm, the MAE remains low at 2.8% for 180 s and 2.7% for 270 s, further reinforcing the model's precision when interpolating. The reason for this relatively low error in the interpolated cases lies in the fact that the model has been trained on data points that fall within this dwell-time range. The PIDL model excels at capturing patterns and trends within the dataset they have been trained on, and when predictions are made within this range, the model is better equipped to accurately estimate the residual stresses. However, when the model is tasked with predicting residual stress at extrapolated dwell times, the accuracy declines significantly. At a build height of 10 mm, the MAE at 450 s rises to 7%, and at 500 s it reaches 10.5%. This trend is observed across all build heights, though the magnitude of the error varies. The sharp increase in MAE for the extrapolated cases can be attributed to the limitations of the PIDL model when making predictions outside the range of the data it was trained on. Extrapolation requires the model to predict values for dwell times that it has not encountered, making the predictions less reliable as the model lacks sufficient knowledge about the underlying relationships between residual stress and dwell time beyond the experimental data range.

Table 5.4: Mean absolute error (in %)-in forward prediction of residual stress at selected dwell-times.

Build height (mm)	Interpolated residual stress (σ_{RS})				Extrapolated residual stress (σ_{RS})			
	180 s (MPa)	MAE (%)	270 s (MPa)	MAE (%)	450 s (MPa)	MAE (%)	500 s (MPa)	MAE (%)
10	273.4	3	240	1.5	386	7	304.5	10.5
20	305.9	2.6	332.2	2.4	316.8	9.6	340.3	6.9
30	358	3.3	325.7	3.5	419.4	7.7	437.2	7
40	550	2.8	572	2.7	628.8	6.6	634.8	9.8

5.3.3 Inverse prediction

Inverse predictions of inter-layer dwell time or inter-pass temperature are conducted based on targeted residual stress values. For predicting temperature, the input includes dwell time and spatial coordinates. Conversely, for predicting dwell times, the model uses residual stress, nodal temperature, and distance along the build direction as key attributes. The residual stress values selected for these predictions are carefully chosen to be below the permissible tensile strength of the material, ensuring structural integrity during the build process of the printed thin wall. In addition, the residual stress values are chosen from the experimental measurement. The DL models (Models 1-5), each with varying architectural configurations, are trained and fitted to the datasets. The performance of these models is assessed based on their ability to accurately predict inter-pass temperatures and dwell times under different stress conditions. By incorporating material properties, build direction coordinates, and residual stress thresholds, the models not only improve prediction accuracy but also ensure that the predicted values stay within the material's safe operational limits, enhancing the overall reliability of the printed structure. For inverse predictions, the optimized PIDL model (Model 5) demonstrated exceptional performance, with an R^2 value of 99.8% and RMSE of 5 seconds for dwell time, and an R^2 value of 99.9% with an RMSE of 2.2°C for temperature predictions. This optimized model is, therefore, well suited for further analysis.

Table 5.5 presents the inverse predictions of inter-layer dwell time (D_{TM}) and inter-pass temperature for mitigating residual stress in a thin wall structure fabricated using the arc-DED process. These predictions, made by a PIDL model, are compared against experimental values at different build heights (10 mm, 20 mm, 30 mm, and 40 mm) and targeted dwell times (180 s, 270 s, 450 s, and 500 s). The PIDL model's performance reveals a clear distinction between its ability to predict dwell time and inter-pass temperature. For dwell time, the model achieves consistently low MAE value, indicating a high degree of accuracy. For instance, at a build height of 10 mm, the MAE for dwell time remains within a narrow range of 0.22% to 0.89% across all dwell times. This pattern is repeated for other build heights, where the MAE for dwell time rarely exceeds 1%. In contrast, the model's prediction for inter-pass temperature shows larger deviations, particularly for extrapolated dwell times. At a build height of 10 mm and an extrapolated dwell time of 500 s, the MAE for temperature rises significantly to 10.6%, while the MAE for dwell time remains stable at 0.22%. Similar discrepancies between temperature and dwell time predictions are observed across all build heights, with temperature errors being consistently higher.

Table 5.5: Mean absolute error (in %)-in inverse prediction of temperature and dwell-time.

Build height t (mm)	$D_{TM} = 180$ s			$D_{TM} = 270$ s			$D_{TM} = 450$ s			$D_{TM} = 500$ s		
	T_{PR} (°C)	MAE (%) for T_{PR}	MAE (%) in D_{TM}	T_{PR} (°C)	MAE (%) for T_{PR}	MAE (%) in D_{TM}	T_{PR} (°C)	MAE (%) for T_{PR}	MAE (%) in D_{TM}	T_{PR} (°C)	MAE (%) for T_{PR}	MAE (%) for D_{TM}
10	45	2	0.3	38	3.6	0.22	25	6	0.89	25	10.6	0.22
20	62	1.9	0.2	40	4.4	0.14	25	6.8	0.62	25	6.2	0.04
30	74	2.7	0.2	47	4	0.26	30	7	0.82	25	9.7	0.34
40	76	3.1	0.2	52	3.8	0.67	30	5.7	0.2	25	8	0.84

To assure high quality and reliable printed thin wall in extreme operating conditions pertaining to the targeted applications, it is required to control residual stress up to a certain

extent. Either the existing methodologies based on pure physical model or complete experiments cannot be utilized as a common practice for evaluation and mitigation of residual stress in a thin wall structure. Here, the optimization of dwell time for multi-layer DED is prerequisite for modulating the residual stress that significantly affects the printing quality. The bidirectional modelling approach proposed here for developing computationally efficient tools can be effectively utilized for elucidating the complex thermo-mechanical behavior and prediction of DED attributes for any other AM processes. The current methodology can act as an intuitive way for the development of an efficient digital twin tool for the development of thin wall structure following DED process.

5.4 Bi-directional scanning strategies for residual stress management

In arc-based DED of 9Cr-1Mo steel, scan-path design governs the thermal history that drives microstructural transformation and residual stress evolution. Unidirectional passes tend to impose asymmetric heat flow and steep longitudinal gradients. Whereas bi-directional scans balance successive heat inputs, moderates cooling rates, and homogenize thermal fields along the build direction. Within this framework, finite-element thermomechanical simulations coupled with non-equilibrium thermodynamic analysis (Scheil–Gulliver) clarify how bi-directional passes suppress δ -ferrite, stabilize a predominantly martensitic matrix, and promote uniform carbide precipitation ($M_{23}C_6$, MX). Microstructural characterization via EBSD (including KAM mapping and phase fraction analysis) and TEM confirms refined martensitic laths, fewer dislocation tangles, and improved precipitate stability under bi-directional strategies, linking thermal gradient control to microstructure–property improvements. Together, these results establish bi-directional scanning as a physically grounded lever for residual stress management and microstructural refinement in ferritic/martensitic steels, offering a practical route to mitigate Type IV cracking and to enhance component reliability for high-temperature service.

5.4.1 Temperature and residual stress

Printed layer experiences complex thermal cycles (rapid heating and cooling) at any spatial location, where the evolution of microstructure and the mechanical properties are directly linked with thermal history. The experimental measurement of thermal history and residual stress on each deposited layer is cumbersome and often requires sophisticated set-up. Hence, a well-tested numerical model analyses the effect of in-situ thermal treatment on distortion, residual stress and microstructural properties. Figure 5.20 shows the comparison of temperature distribution and residual stress evolution at different heat input levels. The thermocouples are spot welded at 10 mm from the interface at fifth layer of deposition. The temperature profiles are extracted up to the 20th layer. Figure 5.20 (a and b) shows 15 distinguished peaks for both the uni-directional and bi-directional deposition strategies at the heat input of 310 J/mm. The maximum temperature gradually reduces on deposition of stack of layers. The relative difference in the maximum temperature after deposition of 6th layer is less than 5%. However, the peak temperature for bi-directional scan (1037°C) is more than that of uni-directional (797°C) scan. For the same dwell-time, the bi-directional scan holds more preheating temperature than uni-directional scan. At the initial phase, the simulated and experimental results align closely, reflecting the accuracy of the model in capturing the thermal response.

While the preheating temperature of the newly deposited layer is approximately the same in all the passes, the same amount of heat dissipation takes place each time from the stack of layers. This preheating effect reduces the residual stress by diminishing the temperature gradients on further deposition of a new layer. The magnitude of this stress is correlated with variation of temperature gradient during the cooling phase. However, the tensile stress in thin-wall structure is highly related to the distortion of the fabricated wall. Both the scanning strategy and the level of heat input have a significant role on the evolution of residual stress. Figure 5.22(c and d) depicts the comparison of computed longitudinal residual stress (S_{11}) with experiments along the deposition direction of substrate. Tensile stress is attributed to the restricted non-uniform contraction on the deposition of successive layers. The maximum contraction along the longitudinal direction creates a higher magnitude of stress as compared to transverse and through thickness component of stresses. Black dotted lines in Figure 5.20c illustrate the point of residual stress measurement along the path. The changes from

compressive to tensile stress is observed at the mid-span of the deposit. The maximum magnitude of tensile stress (~ 276 MPa) for uni-directional path is more than that of bi-directional path (~ 265 MPa). The bi-directional scan produces relatively uniform distribution of temperature gradients on depositing the material. At the low level of heat input, lesser amount of heat accumulation takes place between stacks of layers on deposition of new layer. Hence, the uniform expansion and contraction of the material at surface is expected. Figure 5.22d indicates that compressive residual stress decreases (82 MPa to 60 MPa) and tensile residual stress increases (257 MPa to 280 MPa) with increasing heat input from 232 J/mm to 465 J/mm. It is apparent that the bi-directional path is a better option than uni-directional path at the lowest heat input.

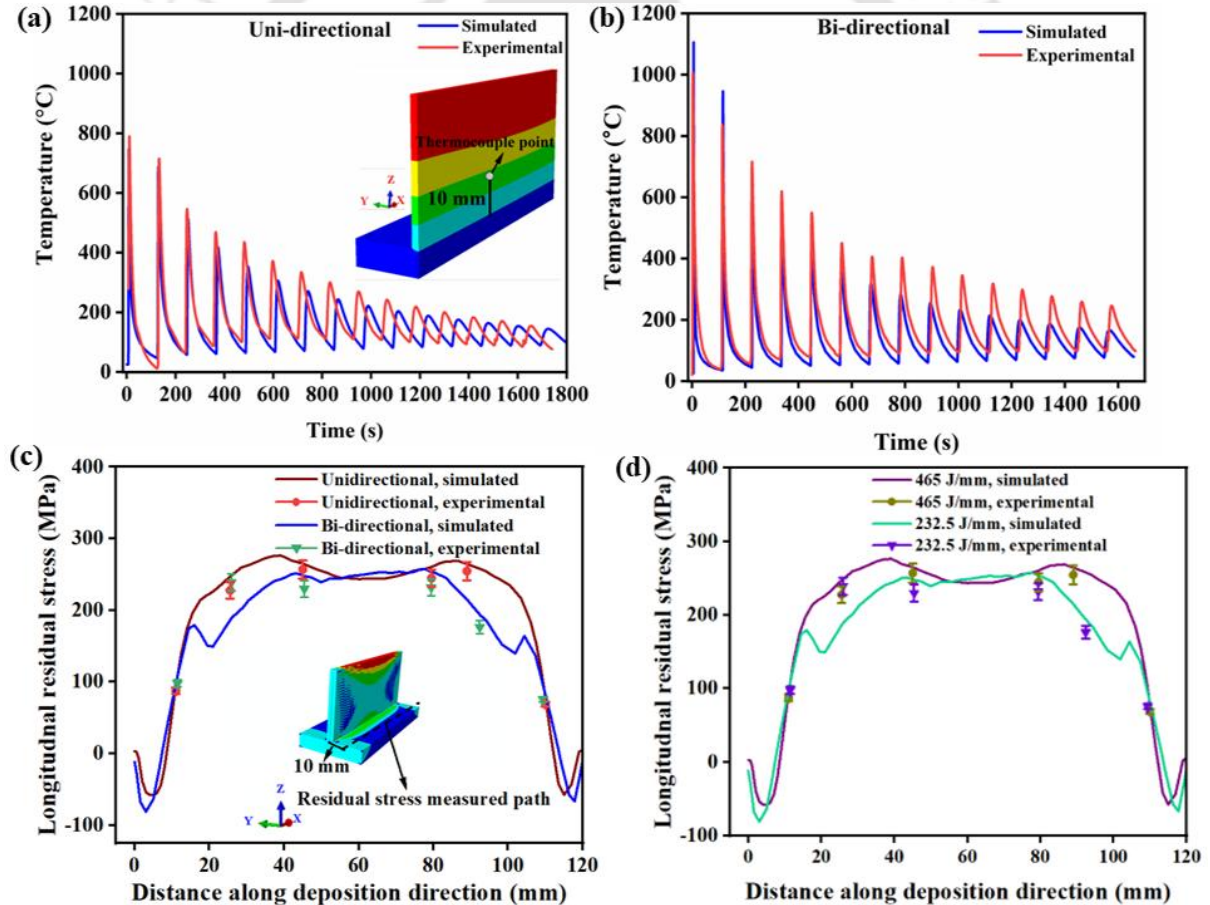


Figure 5.20: (a, b) Comparison of temperature profiles at a heat input of 310 J/mm. (c, d) Residual stress distribution on the 9Cr-1Mo steel substrate under different scanning strategies and heat input levels, highlighting the influence of deposition parameters on stress variation. Error bars in (c, d) represent ± 1 standard deviation, calculated based on experimental data.

The variation in microstructure is directly influenced by the thermal cycle and associated cooling rate. The solidification behavior of the deposited material is governed by the temperature gradient (G) and the growth rate (R). The cooling rate is estimated as $G \times R$. Typically, the maximum growth rate (R) along the deposition velocity vector remains constant, while the temperature gradient is calculated between the liquidus and solidus temperature difference along the deposition velocity vector [35]. Figure 5.21a shows that the cooling rate drops rapidly with the first few layers and, thereafter, it stabilizes. At initial stage, the heat-transfer is dominated by conduction mode along the build direction. With the increase of the number of layers, the convective and radiative modes become more active leading to less heat dissipation and additional preheating effects. However, the cooling rates are significantly higher for bi-directional scan as compared to uni-directional scan. Hence, bi-directional scan is expected to produce more refined microstructure. The cooling rate reduces gradually on subsequent deposition of new layer as depicted in Figure 5.21b. At the mid-of the first layer, the cooling rate of $\sim 2814^{\circ}\text{C/s}$ and 2110°C/s are estimated for both the printing strategies. It is approximately three times more than that of last layer due to balanced effect of direct chilling from cold substrate and the loss of heat from the newly deposits. However, the cooling rate at 20th and 25th layer remain stable ($838 - 873^{\circ}\text{C/s}$), which is attributed to the almost constant heat dissipation (same thermal diffusivity) and maximum heat loss from the exposed surface. The heat accumulation in successive layer formation enhances the peak temperature that act as preheat temperature for the next layer. Hence, the temperature difference reduces with successive layer formation over constant deposition time. Therefore, imparting a new layer always reduces the cooling rate. On enhancing the heat input from 232 J/mm to 465 J/mm , reduction in the cooling rates from 3382°C/s to 1770°C/s are observed. High heat content and peak temperature at 465 J/mm , the cooling period is considerably high that effectively reduces the cooling rate. In the last deposited layer, marginal variation of cooling rate from 800°C/s to 743°C/s is observed.

The effect of scanning strategy and heat input on inter-pass temperature and residual stress are computed at the mid-length of the printed structure along z - z' line (Figure 5.21c). The inter-pass temperature along the build direction for bi-directional scan is higher than uni-directional scan, which facilitates the relaxation of stress after the cooling period of 100 s. At the top of the printed structure, the maximum tensile residual stress is observed as $\sim 581 \text{ MPa}$

for the unidirectional path and ~ 492 MPa for the bi-directional path. The region near this location experiences post-heat treatment like thermal cycles, whereas it is completely absent at the final layer. Figure 5.21d represents the variation of longitudinal residual stress for bi-directional scanning strategy, which is attributed to differential preheat temperature and cooling rate at two extreme heat inputs. Low heat input results in minimum inter-pass temperature and low heat accumulation of the newly deposited layer. It accounts more uniform contractions leading to low magnitude tensile residual stress. When the heat input increases to 465 J/mm, the longitudinal residual stress raises from 264 to 668 MPa. It infers that the low heat input condition is always favorable to produce minimum tensile residual stress.

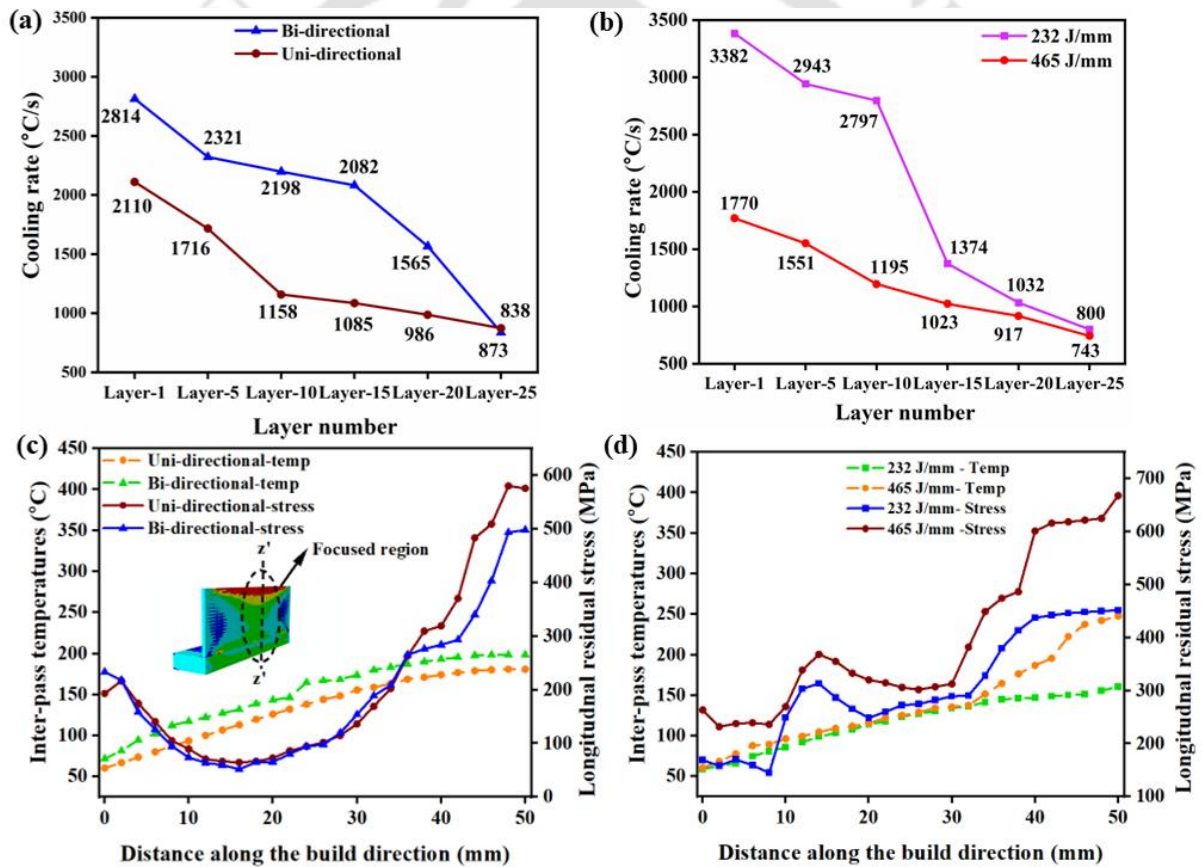


Figure 5.21: (a) Comparison of cooling rates under different printing strategies, illustrating the impact of scanning direction on thermal gradients. (b) Cooling rates observed at the lowest and highest heat input levels for the bi-directional printing strategy. (c) Inter-pass temperature and residual stress distribution for different printing strategies, highlighting variations in

thermal management and stress evolution. (d) Inter-pass temperature and residual stress profiles at the lowest and highest heat input levels for the bi-directional printing strategy.

Figure 5.22 illustrates the variation of longitudinal residual stress at the substrate-deposit interface. This interface experiences non-uniform thermal cycles as per scanning strategy. In the very first layer, the heat is dissipated to the relatively cooler substrate. Overall, the residual stress level decreases with deposition of further layers. The uni-directional scanning confers relatively uniform temperature gradient and stable cooling rates along the interface. This uniformity allows tensile residual stress to gradually decrease from ~ 527 MPa to 330 MPa after the deposition of 25th layer. The steady cooling mitigates stress gradient along the deposition direction and reduces the likelihood of interfacial separation. Bi-directional scanning introduces fluctuating temperature gradient and localized cooling variation, leading to uneven thermal contraction. Although tensile stress still reduces (from ~ 487 MPa to 312 MPa), the alternating thermal loading causes less uniform stress distribution compared to uni-directional scanning. When the scanning strategy changes to bi-directional at the 25th layer, the maximum tensile residual stress decreases from ~ 380 MPa to ~ 300 MPa. Thus, managing the temperature distribution and its gradient along the deposition direction is key to controlling residual stress at the substrate-deposit interface.

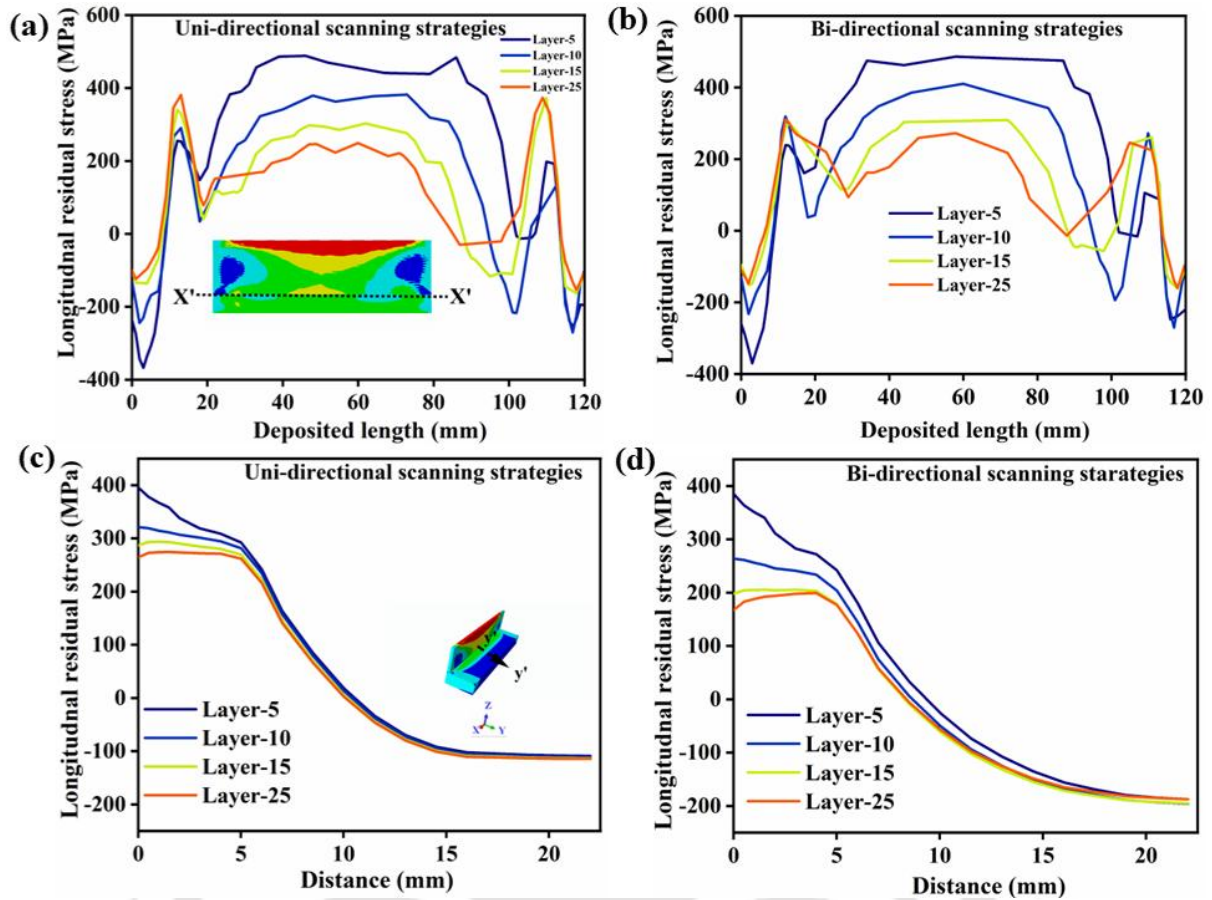


Figure 5.22: Effect of scanning strategies on the evolution of residual stress: (a, b) Residual stress distribution at the interface of the substrate and deposited material. (c, d) Residual stress variation within the substrate material, demonstrating how different scanning strategies influence stress development.

The stress evolution on substrate is significantly affected by the deposition of successive layers, as depicted in Figure 5.22 (c and d). As new layer is added, the residual stress redistributes, and it transits from tensile at the centerline to compressive towards the substrate edge. The substrate acts like a heat sink, where heat dissipation is very high and a steep temperature gradient exists near the deposited layer. Hence, relatively cooler zone tries to reach compressive state of stress. At the 5th layer deposition, the maximum tensile stress on substrate reaches 400 MPa for the uni-directional scanning and 385 MPa for the bi-directional scanning. It is attributed to the substrate's direct exposure to rapid cooling and shrinkage effects, coupled with the limited thermal mass of the deposited layers, which leads to steep thermal gradient. As deposition continues, the gradient becomes less severe due to increased heat accumulation.

By the 25th layer, tensile stress over the substrate significantly decreases (~ 274 MPa for the uni-directional and ~ 180 MPa for bi-directional scanning). Last deposited layers act as thermal buffer that effectively redistribute temperature and lower the gradient and cooling rate and allowing more gradual stress relief. The bi-directional strategy, with its alternating deposition pattern, facilitates further reduction in tensile stress since this strategy helps to distribute heat more evenly, promoting uniform stress relaxation across the substrate.

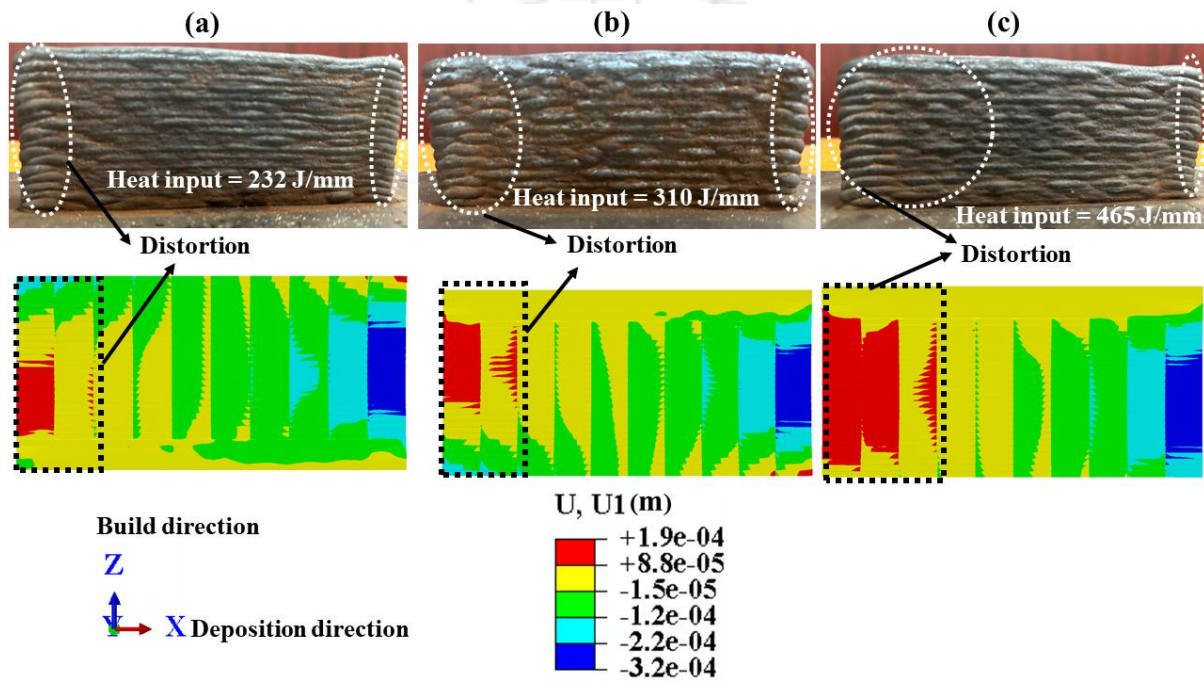


Figure 5.23: Comparison of numerically computed distortions with experimental measurements at different heat input levels: (a) 232 J/mm, (b) 310 J/mm, and (c) 465 J/mm. The results highlight the accuracy of the numerical model in predicting distortions under varying thermal conditions.

Figure 5.23 demonstrates the influence of heat input on deformation pattern of printed structure along the deposition direction. As heat input increases, there is a noticeable rise in longitudinal distortion, highlighted by the black-dotted rectangles in the figure. This distortion is a complex function of thermal expansion and contraction dynamics, heat accumulation, differential cooling, thermal properties of the material, and residual stress formation. At high heat input, larger temperature gradient and slower cooling rate lead to greater thermal stress and plastic deformation. The material's response to these thermal cycles, particularly its

susceptibility to creep and softening, further exacerbates the distortion. The combined effect of these phenomena at high heat input always promotes larger thermal strain and more pronounced longitudinal distortion along the length of the fabricated wall. This distortion can be managed by providing the low heat input.

Understanding the evolution of residual stress and distortion is critical for ensuring the structural integrity and dimensional stability for any layer-by-layer deposition process, specifically for 9Cr-1Mo steel, which is widely used in high-temperature applications. The non-uniform temperature distribution mainly drives the stress evolution and distortion pattern and govern local microstructure formation mainly through phase transformations like δ -ferrite dissolution, martensitic transformation, and carbide precipitation. These microstructural changes directly affect the mechanical properties, including strength and creep resistance, which are critical for the targeted application. FE simulations provide insights into temperature history and stress evolution associated with different scanning strategies. However, complex microstructural behavior of 9Cr-1Mo steel necessitates a detailed understanding of phase transformation from temperature history to establish a direct link between residual stress distribution and microstructure. Thermodynamic modelling is indispensable for predicting phase formation and stability under varying thermal conditions, while experimental analysis of microstructure and mechanical properties validates these predictions and assesses the performance of the material.

5.4.2 Solidification and microstructure

The formation of different phases in the printed wall is analyzed using Thermo-Calc software considering thermodynamic equilibrium of 9Cr-1Mo steel and employing TCFE9 steel database [185]. Figure 5.24a depicts the volumetric phase fractions at thermodynamic equilibrium temperature considering the compositions. The Scheil-Gulliver solidification simulation (Figure 5.24b) predicts the non-equilibrium phases that could appear in the fabricated thin wall structure. This model assumes that the diffusion in the liquid phase is at infinite speed. There is no diffusion within the solid phase, and the solid/liquid interface remains in a state of local thermodynamic equilibrium. δ – ferrite first forms from the liquid phase at relatively high temperature. Consequently, the austenitic phase forms by peritectic reaction ($L + \delta \rightarrow \gamma$). Formation of $M_{23}C_6$ takes place at a temperature less than 872°C. The

MX type precipitation evolves at temperature below 1130°C. The laves phase (Fe_2Mo) begins to develop at temperature below 635°C. The maximum phase fraction for MX and M_{23}C_6 are 2.5% and 1.9%, respectively. It is understood that at equilibrium, δ – phase present in stable condition at relatively high temperature ($>1400^\circ\text{C}$). However, the DED process is associated with non-equilibrium solidification, hence formation of δ – ferrite takes place following non-equilibrium path. Similar inferences are applicable to martensitic steel [186]. High cooling rate in layer-by-layer deposition process leads to the suppression of δ – phase formation and facilitates the direct formation of austenitic phase in cellular or dendritic structure [187]. The findings of this study reinforce this standpoint. In Figure 5.24b, the Scheil-Gulliver solidification path deviates from the equilibrium path. Here, the non-equilibrium solidification still leads to 74% of the δ -ferrite precipitating first from the liquid phase. However, the blending of δ and γ phases within the cellular or dendritic morphology may incorporate the segregation at this high cooling rate [188]. It is important to note that the Scheil-Gulliver model only predicts the diffusional phase transformation. However, during cooling, austenite in 9Cr-1Mo steel further transforms into martensite.

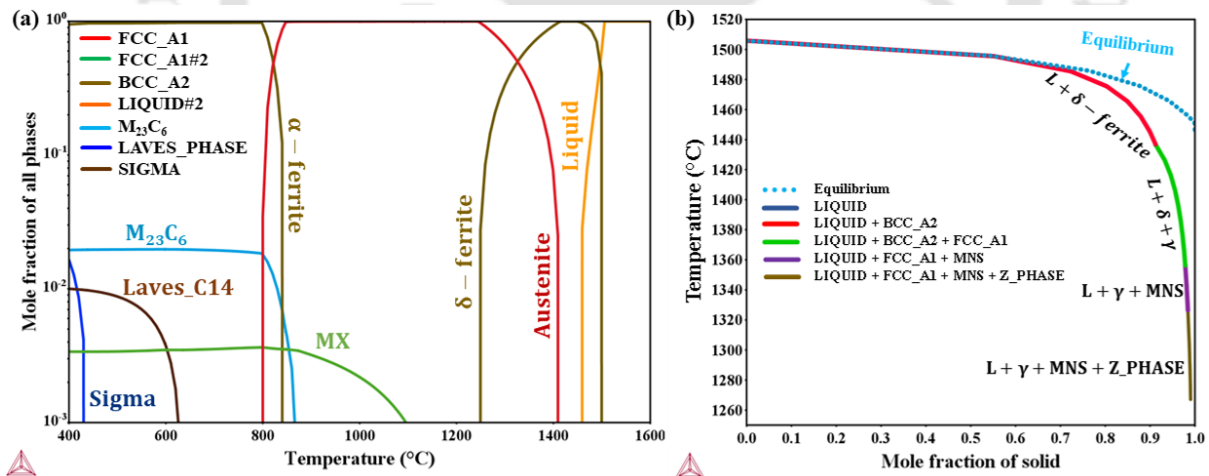


Figure 5.24: Evolution of phases in 9Cr-1Mo steel: (a) Phase fractions under equilibrium conditions, showing the stable phases at different temperatures. (b) Phase evolution predicted using the Scheil-Gulliver model for non-equilibrium conditions, illustrating the effects of rapid cooling on phase transformation during the deposition process.

The macrograph of the deposited layer is depicted in Figure 5.25 a1-a3. It is obvious that the bulk heat transfer between stacked layers governs the overall temperature distribution, while the localized heat transfer significantly influences the microstructural characteristics of the printed sample (Figure 5.25 b1-b3). At the bottom, almost uniform heat dissipation through relatively low material volume exhibits a straight-line profile. In contrast, the free surface of the deposited layer consistently exhibits a parabolic profile due to uneven thermal dissipation at the uppermost layers. The microstructure of the printed component predominantly consists of lath martensite, δ -ferrite, and prior austenitic grain boundaries (PAGBs). Martensitic phases appear as darker regions, while δ -ferrite phases, identifiable as brighter regions, are distributed along build direction (Figure 5.25 b1-b3). The fraction of δ -ferrite decreases from the top to the bottom of the wall, correlating with the cooling rate variations across the build. Relatively high heat dissipation rate at the top region favors formation of δ -ferrite and equiaxed martensitic lath. This refined microstructure is expected to enhance isotropy and improved mechanical properties.

In the middle region, preheating from the underlying layers and post-heating due to newly deposited material creates a complex thermal history. This results in a mixed microstructure of δ -ferrite and martensitic laths, with columnar grains dominating due to reduced cooling rates and extended solidification times. At the bottom, the microstructure primarily consists of columnar martensitic grains formed under uniform cooling conditions, as there is less influence of pre- or post-heating. Figure 5.25 c1-c3 indicates the variation of structural morphology from columnar at the bottom to equiaxed at the top. Overall, the variation in δ -ferrite content and martensitic morphology have direct implication for the stability, hardness, and ductility of the printed part, making precise thermal management critical for practical applications.

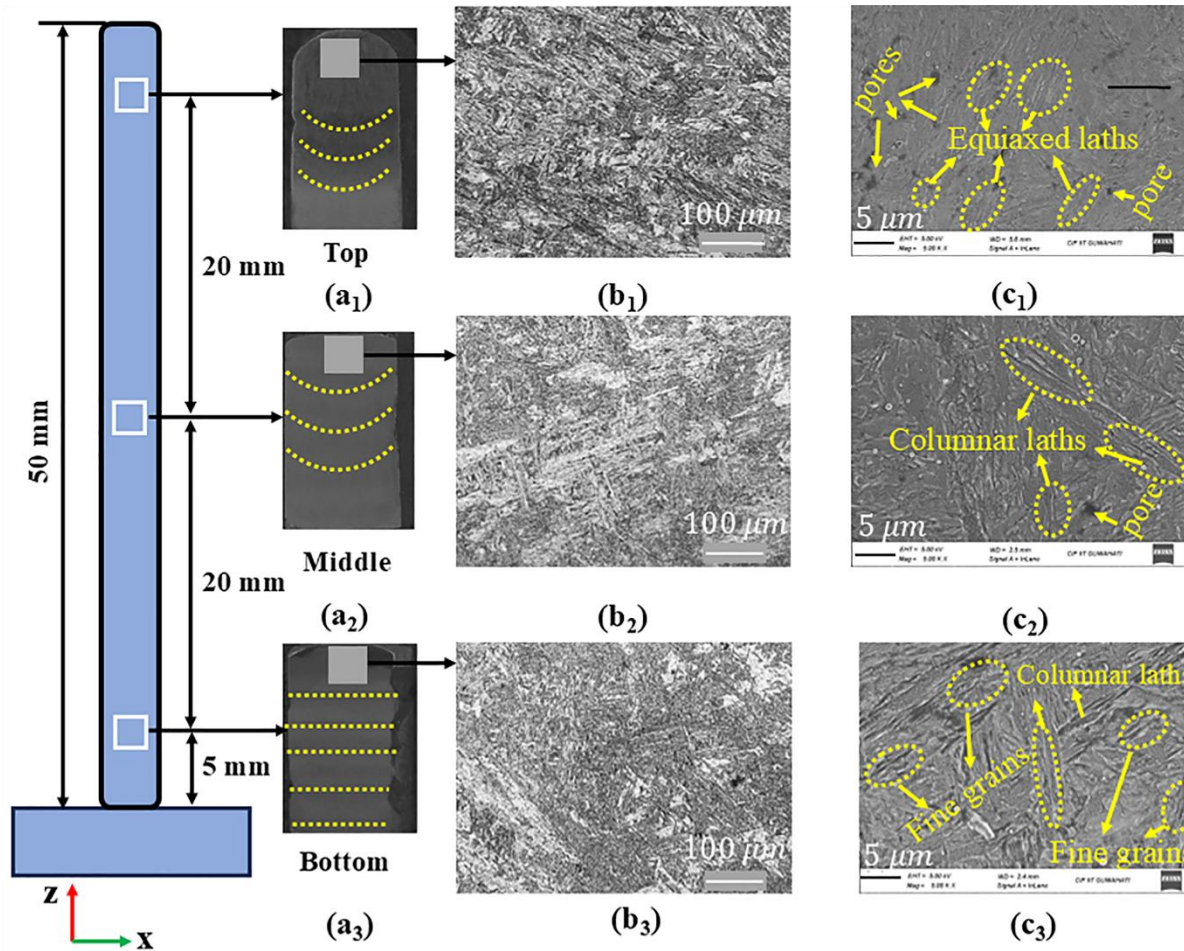


Figure 5.25: Characterization of printed samples at the top, middle, and bottom locations of the wall fabricated using a uni-directional scanning strategy with a heat input of 310 J/mm: (a1–a3) Optical macrographs showing the overall structure at different locations. (b1–b3) Microstructural morphology highlighting grain structures and phase distribution. (c1–c3) Scanning electron microscopy (SEM) images providing detailed visualization of the microstructural features.

The SEM images of the printed samples (extracted from the middle location) using uni-directional and bi-directional scanning strategies are presented in Figure 5.26. The microstructure primarily consists of a ferritic and martensitic matrix with uniformly distributed carbide precipitates. Two types of carbides are observed: MX (M: Nb, V; X: C, N) spherical precipitates, indicated by red arrows, and clusters of $M_{23}C_6$ (M: Fe, Mo, Mn, Cr) carbides, marked by yellow dotted circles (Figure 5.26 a and d). Elemental composition analysis using

Energy Dispersive Spectroscopy (EDS) through point and line scans (Figure 5.26 b and e) reveals weight percentages of Fe, Cr, Mo, Mn, V, and Nb. These results confirm that higher Cr and Mo content drives the formation of $M_{23}C_6$ carbides, while Nb facilitates the formation of MX carbides.

Elemental mapping (Figure 5.26g) further corroborates the presence and distribution of these precipitates. Notably, the average Cr-to-Fe ratio for $M_{23}C_6$ carbides is measured as 0.24 and 0.29 in uni-directional and bi-directional scanning strategies, respectively. It is well aligned with literature reported results [77]. The elevated Cr-content in $M_{23}C_6$ carbide is attributed to elemental partitioning during solidification and subsequent thermal treatment. Cr exhibits a strong affinity for carbon and, hence, it prefers segregating into the $M_{23}C_6$ carbide. This phenomenon ensures stable $M_{23}C_6$ carbide structures, particularly along martensitic lath boundaries, where they play a critical role in enhancing the creep resistance and overall mechanical stability of the alloy [189] Figure 5.26 c and f indicate that Cr enrichment is accompanied by Fe depletion, further validating Cr as the primary component of $M_{23}C_6$ carbide. A more uniform distribution of carbides in bi-directional scanning shows the role of heat input modulation and scanning strategies in promoting microstructural uniformity.

The presence of Cr-based precipitates, such as $M_{23}C_6$ carbides and MX carbonitrides, significantly enhance the mechanical properties of the deposited material by acting as strong barriers to dislocation motion, a primary mechanism of strengthening [190]. Dislocation by these precipitates effectively improves the yield strength and hardness of the alloy. This effect is particularly critical in high-temperature environment, where dislocation movement becomes more prominent. Notably, the density of MX precipitates is higher for the bi-directional printing strategy, further contributing to the material's improved mechanical performance. MX carbonitrides, which preferentially form along martensitic lath boundaries, play a similar role of inhibiting dislocation movement. The enhanced cooling rate of bi-directional scanning promotes the formation of finer precipitates with a higher density. The rapid cooling ensures that alloying elements such as Nb and V precipitate as fine particles. This limited diffusion time suppresses precipitate growth, resulting in nucleation-dominated precipitation rather than growth-dominated. In bi-directional scanning, the finer and more uniformly distributed MX precipitates significantly contribute to grain boundary strengthening and overall mechanical stability.

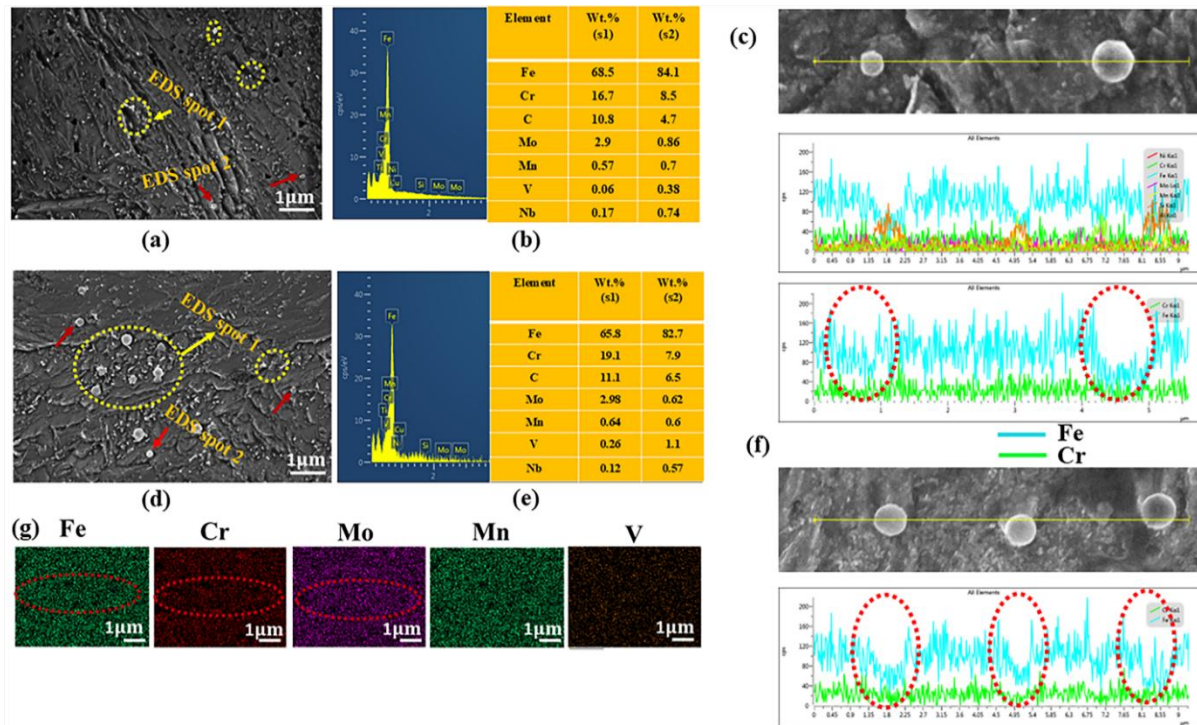


Figure 5.26: Precipitation analysis of printed samples (middle location) fabricated using uni-directional and bi-directional scanning strategies: (a–e) Point scan identifying the available precipitates. (c, f) Line mapping showing the distribution of carbides. (d, g) Elemental mapping of the region enclosing the carbides, illustrating the elemental composition and distribution within the microstructure.

Differences in heat input for bi-directional scanning create significant variation in cooling rates at different locations of the printed walls. Figure 5.27 demonstrates the evolution of the microstructure at varying heat input levels corresponding to different deposit heights along the build direction. The microstructure is almost martensitic for the range of heat input. However, the lath size increases with an increase in the heat input. The presence of δ -ferrite is observed in the middle regions, particularly at higher heat inputs, signifying the effect of slow cooling rate on the formation of δ – ferrite. Figure 5.27 (a, d, g) show that at high heat input, the prolonged cooling period decreases the δ -ferrite content in the upper region, especially in materials like 9Cr-1Mo steel [191]. The lath size is smaller in the bottom and top regions than in the middle. Figure 5.27 (a-c) indicates that the high rate of heat dissipation at the top facilitates almost diffusionless transformation to form martensite. In addition, different

orientation of martensitic lath and δ -ferrite structure is observed at the top and middle locations. In multi-layer thin-wall deposits, the development of larger martensitic laths at the bottom arises from indirect thermal effects and repeated heating during the deposition process. Initially, the bottom layer experiences rapid cooling through conductive heat transfer, resulting in the formation of fine martensitic laths. However, as subsequent layers are deposited, reheating can locally elevate temperature above the austenitization threshold (850°C to 950°C). This leads to the coarsening of prior austenite grain, which, upon re-cooling, transform into larger martensitic structure [192]. Additionally, thermal exposure may trigger recovery phenomena, such as dislocation rearrangement or the merging of sub-laths, further contributing to the apparent coarsening. Hence, the bottom locations exhibit a fully martensitic morphology with fewer MX and $M_{23}C_6$ precipitates (marked with red arrows).

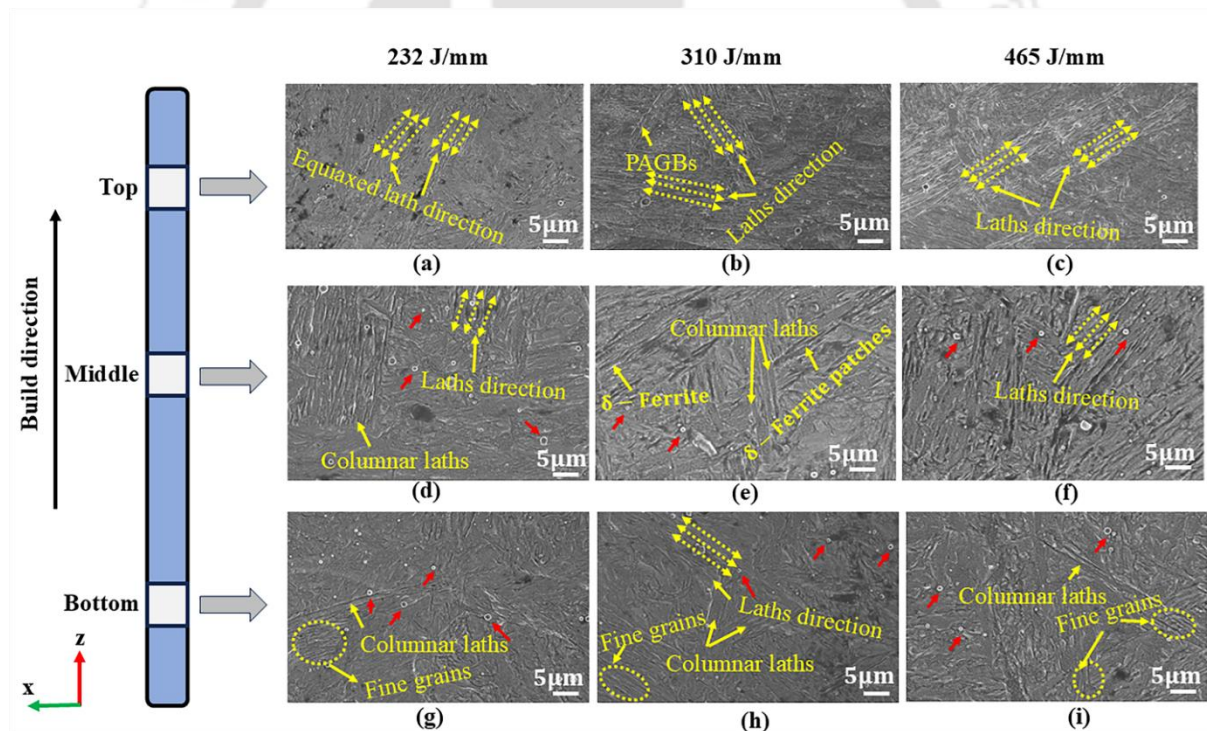


Figure 5.27: Microstructural evolution in the thin-wall structure at different heat input levels: 232 J/mm, 310 J/mm, and 465 J/mm. The samples are extracted from the top (a–c), middle (d–f), and bottom (g–i) regions of the wall, highlighting the variations in microstructure across the build height and heat input levels.

By optimizing heat input, the study provides a practical pathway for addressing critical challenges like mitigating Type IV cracking, especially under the operational conditions of AUSC power plants. Figure 5.27 illustrates the development of equiaxed martensitic laths in the top region and columnar martensitic laths in the middle and bottom regions, which are enhanced by precipitated phases like MX and $M_{23}C_6$. These microstructural arrangements contribute to intergranular cohesion, while the refinement and uniform distribution of laths minimize creep deformation and crack propagation. These phenomena are very common in ferritic/martensitic alloys like P91, P92, and E911 steels. Additionally, prior austenite grain boundaries (PAGBs) present in the structure act as critical barriers to dislocation motion, bolstering creep strength and reducing the risk of Type IV cracking, which originates in the heat-affected zone. The controlled δ -ferrite reduction, especially in the upper region, prevents the formation of weak and creep-prone zones, that ensure enhanced microstructural stability.

The composition of phases in the deposit is analyzed using Rigaku Ultima IV X-ray diffraction techniques, with a scanning speed of $1^\circ/\text{min}$ and a diffraction angle (2θ) range from 20° to 90° . This analysis reveals identical phases at the same diffraction angles for both deposition strategies (Figure 5.28a). At varying heat input, similar diffraction peaks corresponding to the α -ferrite phase with a BCC structure are observed, including crystal planes $\{110\}$, $\{200\}$, and $\{211\}$. However, the analysis could not identify additional phases in the printed samples due to the marginal differences in axis ratios (10^{-4} to 10^{-5}) between ferritic and martensitic structures [193]. In addition, the peaks for the ferrite phases show a slight shift to smaller Bragg angles at different heat input levels (Figure 5.28 c-e). This reduction in Bragg's angle indicates an increase in the spacing between adjacent planes. This study suggests that the lattice constant of the ferritic phase varies due to the presence of solid solution elements in the ferritic matrix during the solidification of the deposited material [10]. The diffraction angles of all these planes do not differ significantly across the samples (44.6° , 44.86° , and 44.64° for (110); 64.8° , 64.86° , and 65° for (200); 82.26° , 82.42° , and 82.5° for (211)). For 9Cr-1Mo material, the martensitic start temperature (M_s) is $380\text{-}400^\circ\text{C}$, and the martensitic finish temperature (M_f) is $200\text{-}230^\circ\text{C}$. It indicates that the austenitic structure within the deposits has sufficient Gibbs energy to transform into a martensitic morphology. Consequently, only a very small percentage of retained austenite, or almost none, is detected

in nuclear-grade steel. However, the diffraction peaks of other intermetallic phases are not observed (There might be bare minimal presence).

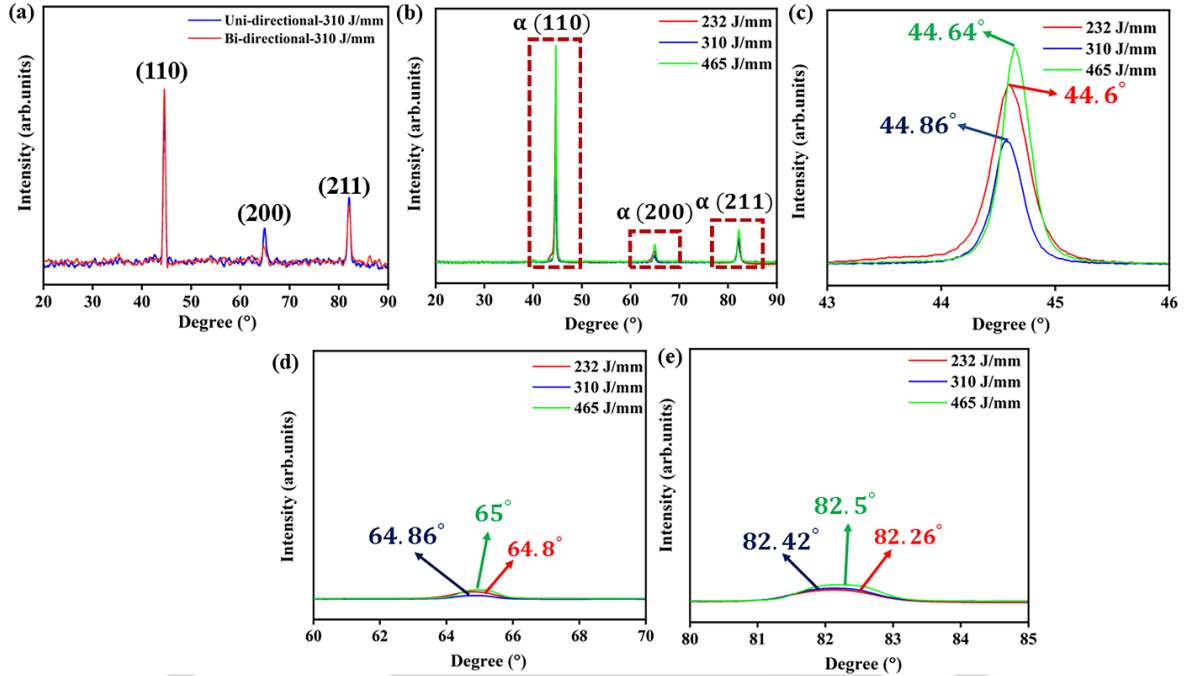


Figure 5.28: X-ray diffraction (XRD) analysis of samples extracted from the middle location of the fabricated walls: (a) Phase distribution in uni-directional and bi-directional deposits at a heat input of 310 J/mm. (b) Effect of different heat input levels on the diffraction patterns, showing variations in phase composition. Magnified views of the (110), (200), and (211) peaks, respectively, providing detailed insights into the crystallographic orientation and phase evolution.

The SEM analysis reveals that the middle locations of the deposits consist of both martensitic and ferritic phases. Further, EBSD analysis is performed on samples extracted from the middle locations for both scanning strategies at a heat input of 310 J/mm (Figure 5.29). The inverse pole figure (IPF) maps (Figure 5.29 a-b) show larger martensitic laths with strong texture orientation in the $\{001\}$ and $\{111\}$ planes, indicating heterogeneity between the δ -ferrite and martensitic phases in the BCC_A2 and BCT configurations. Additionally, MX precipitates are observed as smaller dots dispersed throughout the microstructure. The phase fraction maps (Figure 5.29 c-d) show that the volumetric fraction of martensite is higher for the uni-directional path (99.5%) compared to the bi-directional path (97.5%). This difference

arises from the relatively lower inter-pass temperature in the uni-directional scan, which facilitates the complete transformation of austenite to martensite. However, the high percentage of martensite in the uni-directional deposits contributes to significant volumetric strain, resulting in higher residual stress level. This is further compounded by the high dislocation density in the martensitic structure, leading to severe grain distortion. It is characterised by a lower image quality (IQ) value, as shown in Figure 5.29f. In contrast, the δ -ferrite phase, appearing bright in the IQ map, exhibits higher image quality and low dislocation density. This signifies a relatively lower level of residual stress.

Uni-directional scanning strategy, a higher number of high-angle grain boundaries (HAGBs) are observed compared to the bi-directional strategy, indicating a greater magnitude of residual stress. This observation is consistent with numerical simulations, which demonstrate that the bi-directional path effectively minimizes thermal gradients and mitigates residual stress. The reduced martensitic fraction and dislocation density in the bi-directional scan contribute to lower residual stress levels, improved microstructural uniformity, and enhanced mechanical stability. The Kernel Average Misorientation (KAM) map provides detailed insight into the distribution of local misorientation within the material's grain structure, influenced by residual stress, dislocation density, and the thermal history of the material. In the context of arc-based DED, the choice of scanning strategy significantly impacts these factors, leading to observable differences in KAM fractions. For the uni-directional scan, a higher KAM fraction of 0.99 (Figure 5.29g) is recorded, compared to 0.92 for the bi-directional scan (Figure 5.29h). This indicates that the uni-directional scanning strategy results in increased residual stress, higher dislocation density, and uneven cooling, which collectively lead to greater grain misorientation. In contrast, the bi-directional scanning strategy promotes more uniform heat distribution and cooling, minimizes thermal gradients and residual stress, and reduces dislocation density. Consequently, the lower KAM value for the bi-directional scan reflects improved microstructural stability at reduced deformation, making it a superior choice for achieving consistent and reliable mechanical properties in AM components.

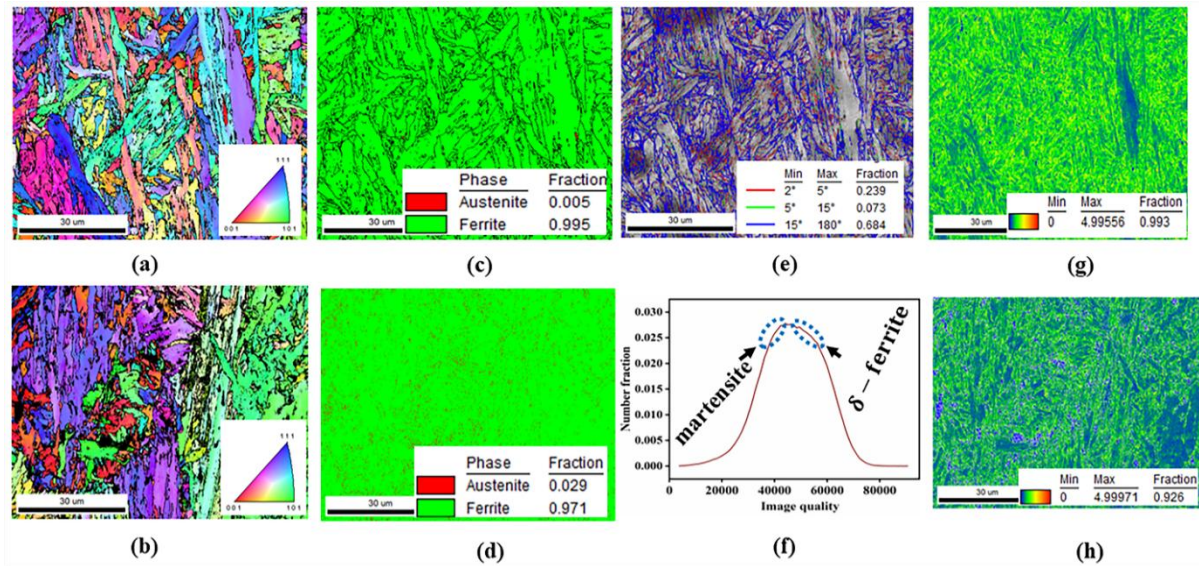


Figure 5.29: Electron backscatter diffraction (EBSD) analysis of deposits extracted from the middle location of the wall printed using uni-directional and bi-directional scanning strategies at a heat input of 310 J/mm: (a, b) Inverse pole figure (IPF) maps showing crystallographic orientation. (c, d) Phase maps illustrating the distribution of phases within the microstructure. (e) Grain boundary map highlighting the boundaries between grains. (f) Image quality variation corresponding to (a). (g, h) Kernel average misorientation (KAM) maps providing insights into the local misorientation and residual strain distribution.

The microstructural morphology at different heat inputs is further investigated by EBSD maps, illustrated in Figure 5.30. The IQ map shows that coarsening of martensitic laths occurs with increased heat input during deposition, Figure 5.30 (a-c). This coarsening is primarily driven by higher atomic diffusion facilitated by prolonged thermal exposure. As heat input rises, the elevated temperature increases atomic mobility, allowing dislocations within martensitic laths to rearrange and annihilate. This reduction in dislocation density leads to the growth and coarsening of martensitic laths, resulting in larger, more relaxed structures. Additionally, analysis is performed for sample extracted from middle location of the deposits that experience repeated heating from subsequent deposit passes, creating an *in-situ* tempering effect. This tempering stabilizes the martensitic microstructure, reduces internal stress and further promotes lath coarsening. The tempering process facilitates dislocation recovery, accelerating the coarsening of laths. Moreover, the IQ map reveals the presence of δ -ferrite, which forms alongside martensitic laths at high heat inputs. The δ -ferrite, with its lower

dislocation density, contributes to further microstructural relaxation, enhancing the coarsening process of adjacent martensitic laths.

The Inverse Pole Figure (IPF) map serves a complementary and essential role by revealing the crystallographic orientation of grains, which cannot be discerned from IQ map alone. The IPF map provides specific insight into the texture and orientation of martensitic laths and δ -ferrite grains, which are key factors in understanding mechanical properties like anisotropy, strength, and stress distribution. As heat input increases, the IPF maps in Figure 5.30 (d-f) show the grain coarsening and reorientation in $\{001\}$, $\{101\}$, and $\{111\}$ in the deposits. Higher heat input enhances atomic mobility, promoting realignment, particularly in the $\{001\}$ plane, which is beneficial for creep resistance. The *in-situ* tempering effect from repeated thermal cycles encourages more uniform grain orientations due to stress relaxation, reflected in the IPF map. This reorientation affects the mechanical properties such as in the $\{111\}$ plane improving ductility and helping accommodate residual stress, complementing the structural changes observed in the IQ map.

Figure 5.30 (g-i) depicts the grain boundary (GB) maps for all the samples. In these maps, low-angle grain boundaries (LAGBs) are represented in red ($2-5^\circ$), while high-angle grain boundaries (HAGBs) are shown in blue ($15-180^\circ$). LAGBs have a minimal impact on dislocation movement and facilitates to prevent the formation of intergranular cracks [194]. Conversely, HAGBs offer substantial resistance to plastic deformation due to the resistance to dislocation movement. The higher number of HAGBs is associated with the finer grain size and the reduced presence of LAGBs, which arise from dislocations generated in the austenite to martensite transformation in the deposit. As heat input increases, the proportion of high-angle grain boundaries (HAGBs) drop from 78.1% to 58.1%. This reduction is attributed to the larger prior austenite grain size, driven by the slower cooling rate of the deposited material. The development of unstable HAGBs, caused by elevated energy across grain boundaries, increases the probability of intergranular fractures at the junctions of successive deposited layers.

Phase maps of samples at different heat input levels are displayed in Figure 5.30 (j-l). The martensitic fraction in each deposit is greater than 90%, with the remainder consisting of retained austenite (RA). When the inter-pass temperature is kept below the martensite start temperature (M_s), fresh martensite and some RA form in the deposited layer because the

martensite finish temperature (M_f) is lower than room temperature. As each new layer is deposited, it acts as a heat source culminating into heat treatment of the layer beneath it. If the temperature surpasses the ferrite to austenite transformation temperature, the martensite converts back to austenite, while regions that don't reach this temperature are tempered. Consequently, for carbon bearing 9Cr-1Mo steel, inter-pass temperature below M_s leads to a non-uniform microstructure and thus uneven properties, whereas temperature above M_s result in more uniform and consistent properties. Since the interlayer temperatures for all heat input conditions are lower than the M_s of 9Cr-1Mo deposits ($M_s \sim 400^\circ\text{C}$), the austenitic phase is fully transformed into martensite. Due to this complex interplay of reheating and cooling as well as the temperature gradient along the build direction, the microstructural evolution and its complexity is very high. The phase fractions of RA under three heat input conditions are 1%, 6.4%, and 7.3%, respectively. These values align with the XRD analysis. The increase in maximum post-heating temperature with higher heat input causes a higher RA fraction in the middle region. At low heat input, the post-heating temperature is below the austenization temperature range, the thermal cycles act as a tempered heat treatment to the previously deposited material. Consequently, martensite formed at the start of deposition is converted to austenite at further heating and afterward it back to martensitic structure. Figure 5.30 (m-o) shows the reduction in KAM value from 0.98 to 0.94 with an increase in heat input. High heat input is associated with more thermal energy, which facilitates atomic movement and promotes the rearrangement and annihilation of dislocations. This reduction in dislocation density is associated with a more relaxed microstructure. In contrast, the residual stress increases with increase in heat input. High heat input intensifies the thermal expansion and contraction cycles. These thermal strains, combined with phase transformations from austenite to martensite (which increases volume), result in greater volumetric strain and, subsequently, higher residual stress. Thus, the dominating mechanism of macroscale thermal strain over low dislocation density (lower KAM values) enhances the residual stress at high heat input. This observation aligns with numerical simulations, which also indicate heightened residual stress along the build direction at the mid-span of the deposits.

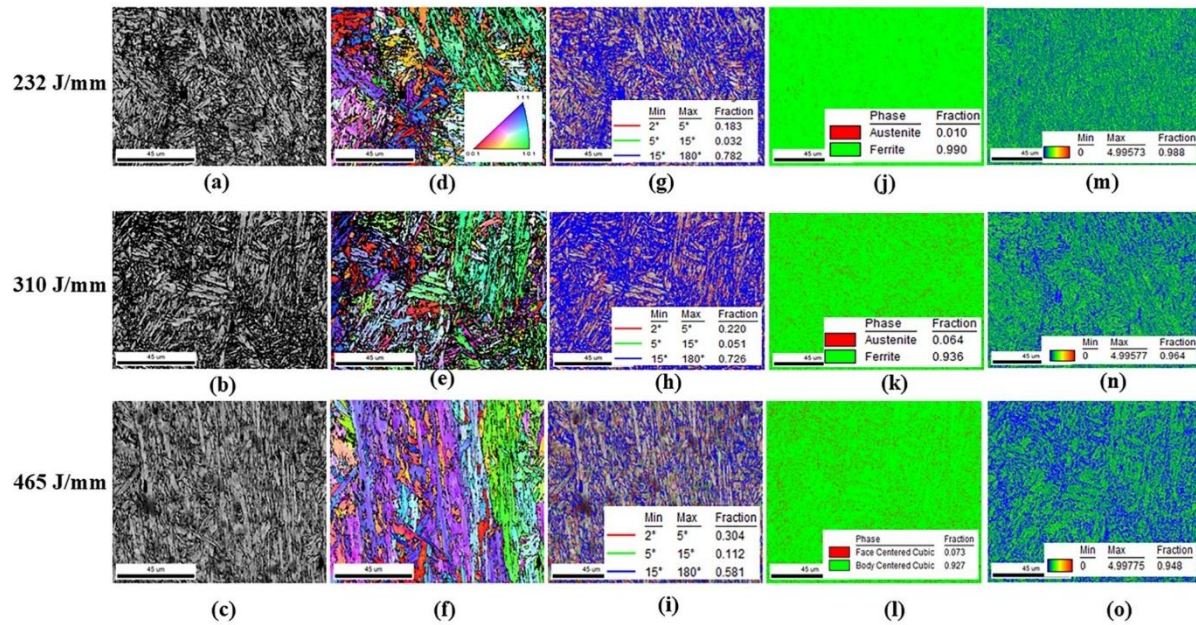


Figure 5.30: Microstructural characterization of deposits extracted from the middle location of the wall using EBSD analysis at varying heat input levels: (a-c) Image quality (IQ) maps showing variations in crystallographic quality. (d-f) IPF map illustrating the crystallographic orientation of martensitic grain. (g-i) Grain boundary map highlights the distribution and types of grain boundaries. (j-l) Phase map showing the distribution of phases within the microstructures. (m-o) Kernel average misorientation (KAM) maps provides insights into local misorientation and residual strain across the microstructure.

Figure 5.31 presents the pole figures of the martensitic phase (BCT configuration) for printed samples fabricated under different heat inputs, illustrating the texture density along the $\{001\}$ plane. The measured texture intensities are 13.4 at 210 J/mm, 4.9 at 310 J/mm, and 2.5 at 465 J/mm, indicating a progressive reduction in preferential crystallographic orientation with increasing heat input. At the lowest heat input (210 J/mm), the relatively high cooling rate leads to a steep thermal gradient and a directional solidification front, which promotes the development of fine columnar martensitic grains aligned along the build direction. Although the grains are refined, their growth remains directionally constrained by heat flow, resulting in a strong alignment of the $\{001\}$ planes and hence a high texture intensity. As the heat input increases to 310 J/mm and 465 J/mm, the cooling rate decreases and the thermal gradient becomes less pronounced. This allows competitive grain growth and partial breakdown of

directional solidification, leading to reduced crystallographic alignment and lower texture intensity. At the highest heat input (465 J/mm), the prolonged thermal exposure and slower cooling facilitate the growth of coarser columnar grains with increased orientation scatter, particularly with respect to the {001} planes, thereby diluting the overall texture strength. Thus, the observed reduction in texture intensity with increasing heat input is attributed to the weakening of directional solidification conditions and increased grain orientation dispersion, rather than equiaxed grain formation.

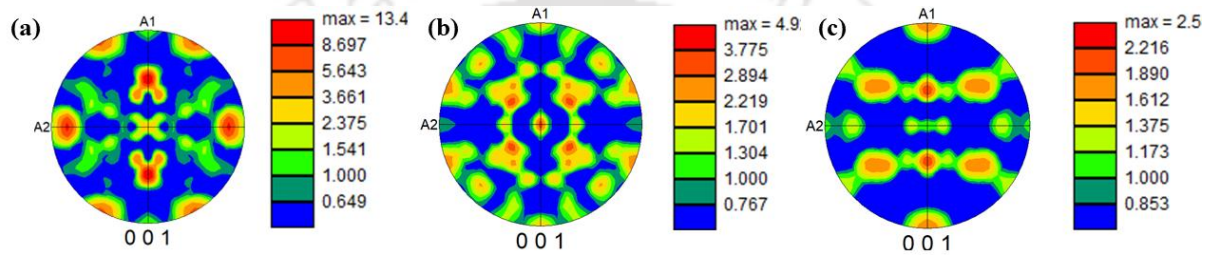


Figure 5.31: Pole figures illustrating the crystallographic texture of deposits at different heat input levels: (a) 210 J/mm, (b) 310 J/mm, and (c) 465 J/mm. The pole figures provide insights into the preferred orientation of grains and the effect of heat input on the development of texture in the microstructure.

Figure 5.32 provides a detailed view of the TEM and selected area diffraction patterns (SAED) of deposited 9Cr-1Mo steel. The microstructure corresponding to the uni-directional scanning strategy (Figure 5.32 a) reveals the presence of martensitic laths, tempered martensitic laths, dislocation tangles, and MX precipitates. The martensitic laths, highlighted in blue, range in length from 1.8 μm to 2.2 μm , while the tempered martensitic laths (marked in green) measured as $\sim 2.24 \mu\text{m}$ in length. These tempered laths form due to local reheating in subsequent deposition of layers, which facilitates tempering of freshly formed martensite and the precipitation of carbides. However, the reheating phase is less pronounced in uni-directional scanning strategy, where it shows limited tempered martensite. Significant dislocation tangles (highlighted in yellow) are observed in the uni-directional samples. A wide range of cooling temperature after solidification (without much reheating effect) is associated with increased lattice strain and residual stress concentration. The localized non uniform temperature gradient in uni-directional scanning imposes high density of dislocation. The MX

precipitates (marked in red) measured as $\sim 50 - 100$ nm indicates the rapid cooling has limited their coarsening. Figure 5.32 b presents the corresponding SAED pattern for the same region shown in Figure 5.32 a, analyzed using CrysTBox software [38]. The SAED analysis confirms the presence of the martensitic BCC phase, with distinct reflections from the $\{110\}$ and $\{200\}$ planes exhibiting d-spacing of 0.202 nm and 0.144 nm, respectively. Zonal axis for SAED patterns are $[2-21]$ (for uni-directional) and $[142]$ (for bi-directional). These reflections verify the presence of martensitic laths in the microstructure. Additionally, reflection corresponding to $M_{23}C_6$ carbides are observed, with d-spacing of 0.128 nm from the $\{220\}$ plane. These carbides, typically precipitated at the martensitic lath boundaries, enhance the hardness and mechanical stability of the tempered regions. Notably, elongated diffraction spots in the SAED pattern indicate strain-induced lattice distortions caused by dislocation tangles. These distortions reflect the high residual stress characteristic of the uni-directional scanning strategy, highlighting the significant thermal and mechanical challenges imposed during deposition. In contrast, Figure 5.32c, corresponding to the bi-directional scanning strategy, reveals a more refined and uniform microstructural arrangement. The martensitic laths in this region exhibit a consistent length of approximately 1.8 μm . The bi-directional scanning strategy, which alternates the heat source direction between layers, promotes more uniform thermal distribution and reduces sharp thermal gradients. This results in controlled cooling rates, facilitating consistent martensitic transformation and refinement of the microstructure. The alternating heat input boosts the formation of tempered martensitic laths ($\sim 1.8 \mu\text{m}$) during the deposition of subsequent layers. These tempered regions play a critical role in reducing residual stress by enabling carbide precipitation (say $M_{23}C_6$). While dislocation tangles are still observed in the bi-directional scanning region (Figure 5.32c), they are significantly less pronounced compared to the uni-directional scanning strategy. This reduction in dislocation density is attributed to the more uniform thermal distribution and minimized thermal gradients inherent to bi-directional scanning. The decrease in dislocation tangles correlates with reduced lattice strain, as evidenced by the corresponding SAED pattern (Figure 5.32d). The diffraction pattern confirms the presence of the martensitic BCC phase, with clear reflections from the $\{110\}$ and $\{200\}$ planes. The corresponding d-spacings of 0.202 nm and 0.144 nm validate the martensitic nature of the observed laths.

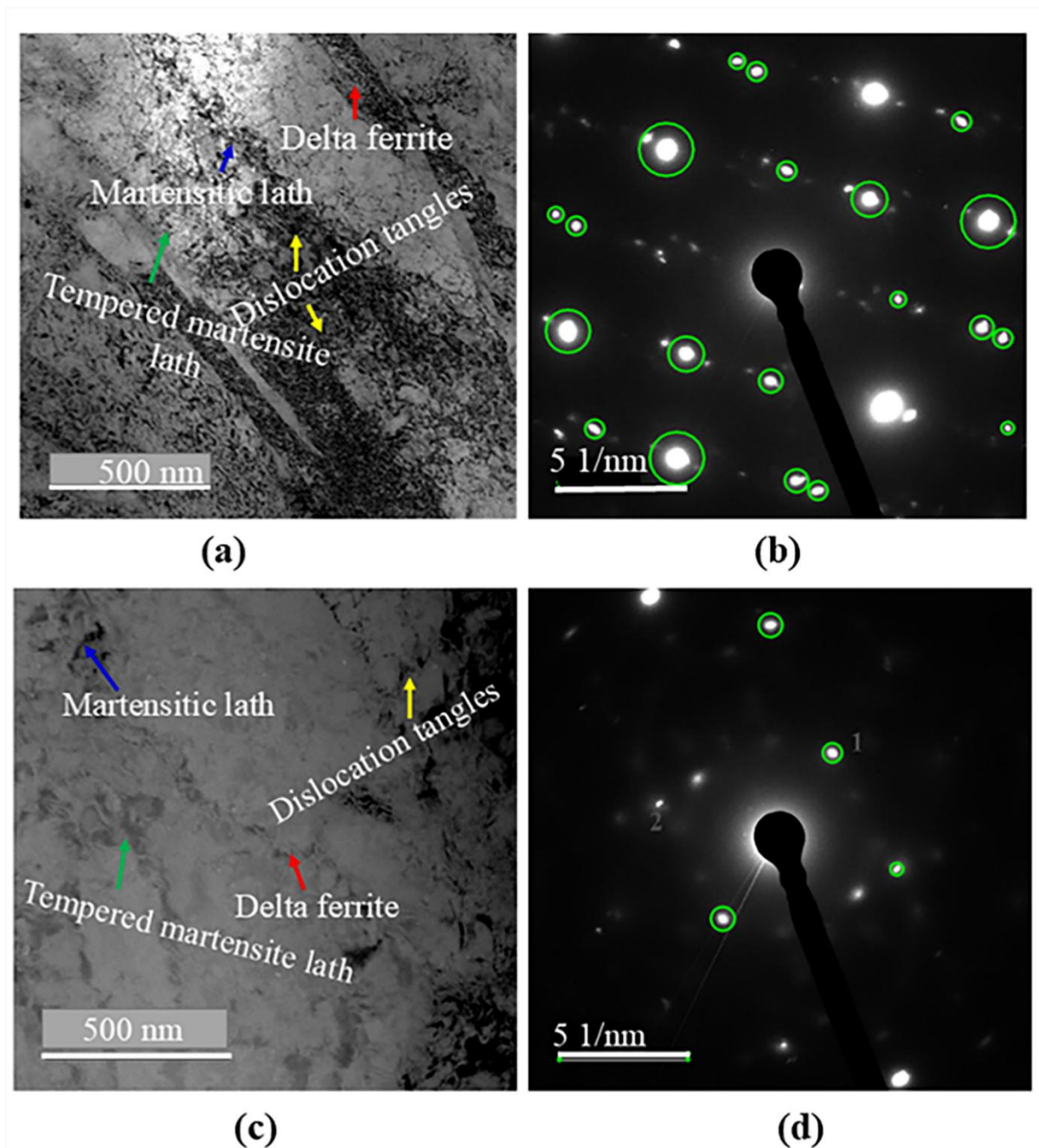


Figure 5.32: Transmission electron microscopy (TEM) morphology of printed 9Cr-1Mo steel extracted from the middle location of the fabricated structure: Comparison of microstructural features for uni-directional and bi-directional scanning strategies, highlighting differences in lath morphology, dislocation density, and precipitate distribution.

Reflections from $M_{23}C_6$ carbides are also detected in the SAED pattern, with d-spacings of 0.128 nm, confirming the presence of these carbides at the boundaries of martensitic and

tempered martensitic laths. These carbides contribute to improved hardness and stability of the tempered regions. Notably, the diffraction spots in Figure 5.32d appear less elongated compared to those in Figure 5.32b, indicating reduced lattice strain and residual stress. This reduction can be directly attributed to the bi-directional scanning strategy, which ensures more even thermal distribution across the layers. The minimized residual stress and reduced formation of dislocation tangles and lattice distortions highlight the advantage of bi-directional scanning in achieving superior microstructural stability and mechanical reliability.

5.4.3 Assessment of mechanical properties

Figure 5.33 illustrates the impact of different deposition strategies on the mechanical properties of 9Cr-1Mo steel fabricated using the DED process. It is important to note that the tensile samples are extracted from the middle region of the printed thin wall structures. Both uni-directional and bi-directional scanning strategies result in printed samples with enhanced tensile properties compared to base material (Figure 5.33 a). However, the printed sample exhibits lower ductility compared to wrought steel. This may be due to the formation of strong texture orientation, non-uniform microstructural content, and debonding between layers. The bi-directional deposits demonstrate superior ultimate tensile strength (UTS) of 1287 MPa and yield strength (YS) of 951 MPa (Table 5.6), exceeding the properties of the base material. This improvement can be attributed to the high density of MX precipitates and refined microstructures resulting from relatively uniform heat distribution in the bi-directional strategy. These favorable conditions coupled with the reduced dislocation tangles enhance grain boundary strengthening. In contrast, uni-directional deposits exhibit relatively lower UTS (1025 MPa) and YS (900 MPa) compared to bi-directional deposits. A wide temperature difference between two successive layers in uni-directional scanning promotes reduced precipitation of strengthening phases. However, the uni-directional deposit displays slightly improved ductility relative to bi-directional deposit. This enhanced ductility can be linked to the alignment of grains in a single direction, facilitated by the uni-directional heat flow, which allows easier deformation along the grain alignment during tensile loading.

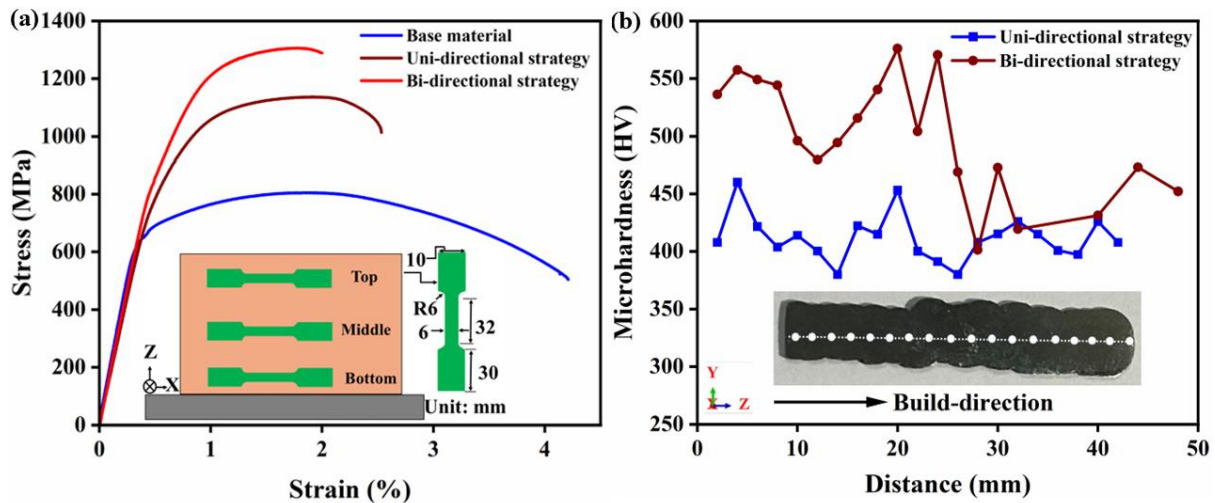


Figure 5.33: Comparison of the mechanical properties of printed walls fabricated using uni-directional and bi-directional scanning strategies at a heat input of 310 J/mm: (a) Engineering stress-strain curves showing differences in tensile behavior. (b) Micro-hardness profiles measured along the build height, highlighting variations in hardness due to differences in scanning strategies and associated thermal effects.

Change in grain growth direction associated with the bi-directional scanning strategy is attributed to improved inter-layer bonding [195]. This alternating scanning path reverses the direction of heat flow between layers, causing grains in adjacent layers to grow perpendicularly to each other. This grain alignment enhances inter-layer cohesion and contributes to the superior mechanical properties observed in bi-directional deposits. Figure 5.33b illustrates the Vickers hardness distribution along the centre line of the deposit. The hardness is the highest near the bottom and progressively decreases toward the middle and top of the deposits. The higher hardness at the bottom is primarily due to rapid cooling rates, which promote the formation of a fine-grained martensitic microstructure. In contrast, slower cooling rates in the top layers lead to grain coarsening and the formation of softer phases such as ferrite and bainite, reducing hardness. Additionally, the repeated thermal cycles during deposition induce tempering of the martensite in the lower layers, further contributing to the reduction in hardness across the build height. The bi-directional scanning strategy demonstrates better control over thermal gradients, resulting in more uniform hardness distribution compared to the uni-directional strategy. Overall, bi-directional scanning exhibits greater uniformity, with a significant (~22%) reduction in hardness from the bottom to the middle region and only minor

(~3%) variation at the top. In contrast, the uni-directional strategy results in more pronounced hardness variation due to wide variation of thermal cycles. This variation is linked to a decrease in dislocation density in regions experiencing high residual stress, as observed in the KAM analysis. The alternating heat input in bi-directional scanning mitigates these effects by promoting more uniform microstructural evolution and residual stress distribution, underscoring its superiority for applications requiring consistent mechanical properties.

Table 5.6: Resemblance of the tensile properties for printed thin wall structures and standard 9Cr-1Mo plate.

Description of Tensile samples	0.2% YS (MPa)	UTS (MPa)	Elongation (%)
Base material	700±18	805±22	4.3±0.3
Uni-directional	887±25	1170±30	2.7±0.2
Bi-directional	951±28	1287±35	2±0.2

The tensile properties of the fabricated walls at different locations (top, middle and bottom) and at different heat inputs using the bi-directional scanning method are shown in Figure 5.34 (a-c). At the lowest heat input level (232.5 J/mm), the top region of the build structure exhibits superior mechanical performance, characterized by a peak ultimate tensile strength of 1221 MPa and the highest elongation of 2.6% (Table 5.7). This can be attributed to accelerated cooling rates and minimal thermal exposure during deposition, which help preserve the integrity of the martensitic microstructure. This is primarily attributed to rapid cooling and minimal thermal cycling in the upper layers, which promote the formation of a fine martensitic microstructure with limited tempering. The reduced thermal exposure helps retain lath sharpness and high dislocation density, contributing to both enhanced strength and ductility. Conversely, the middle and bottom regions are exposed to cumulative heat and multiple thermal cycles, resulting in progressive martensite tempering, coarsening of carbides, and grain growth factors that diminish both UTS and ductility [196]. At the intermediate heat input of 310 J/mm, the middle section of the build exhibits an unexpectedly high ultimate tensile strength of 1285 MPa. This anomalous increase may be linked to localized thermal conditions

that favour the stabilization of retained austenite or the formation of a refined distribution of martensitic variants. While at the highest applied heat input (465 J/mm), the thermal distribution across the build height appears more even, resulting in a nearly uniform UTS of approximately 1210 MPa from top to bottom. A marginal improvement in ductility is also observed, with elongation increasing slightly from 2.0% at the top to 2.15% at the bottom.

Figure 5.34d illustrates the distribution of hardness at various heat inputs. Increasing heat input leads to an average hardness decrease of 27% from the bottom to the top of the fabricated parts. This variation of hardness is mainly driven by the interplay of cooling rates, residual stresses, and the microstructural evolution revealed by KAM maps. The faster cooling rates at the bottom result in fine, hard martensitic or bainitic microstructures, with higher dislocation densities and compressive residual stress contributing to high hardness. When heat input increases (cooling rate slows), the grain coarsens, the formation of softer phases, lower dislocation densities, and tensile residual stress, all of which contribute to reduced hardness in the upper layers. KAM maps visually confirmed this evolution, showing a decrease in local misorientation and dislocation density from bottom to top, further explaining the decrease in hardness. According to the ASTM A335/A335M-21a standard for ferritic steel (9Cr-1Mo) used in high-temperature applications, the required hardness range for boiler components is 195 to 265 HV, which is achieved in the present case. However, the best mechanical properties are achieved at a heat input of 310 J/mm using the bi-directional scanning strategy.

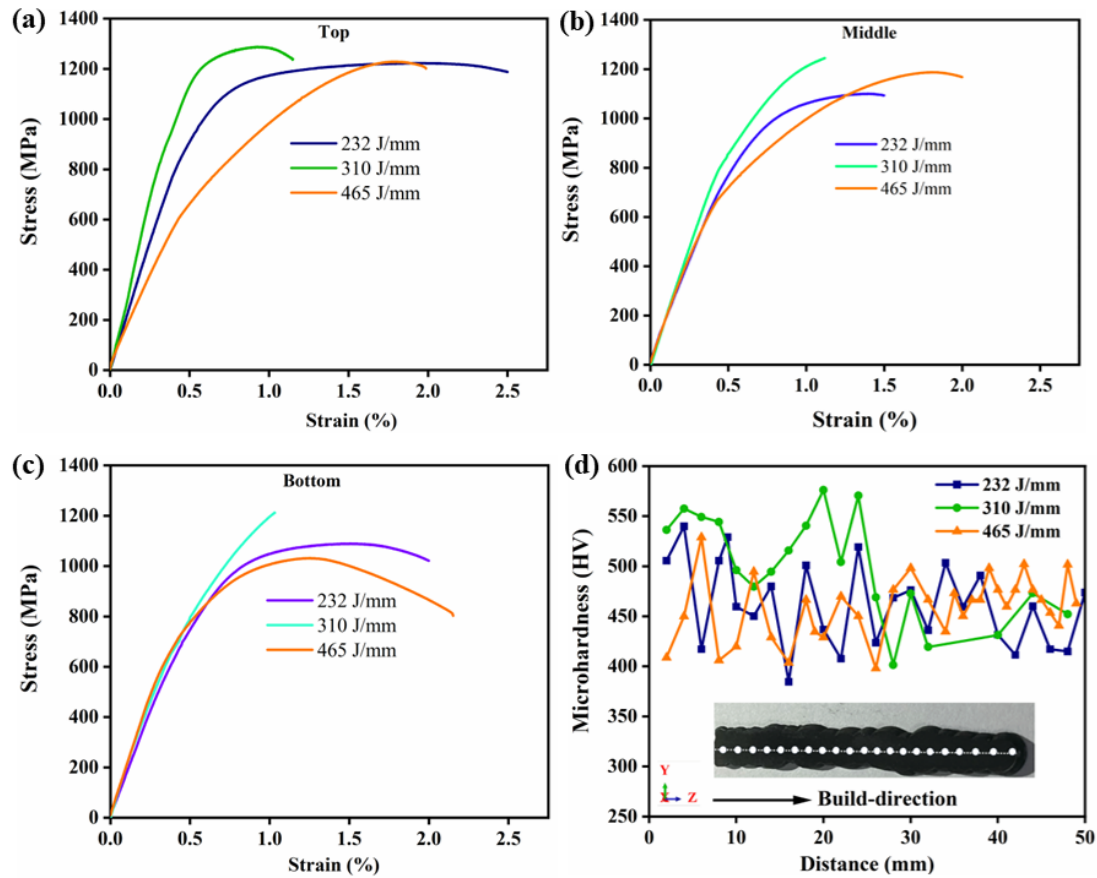


Figure 5.34: Comparison of the mechanical properties of printed walls fabricated using the bi-directional scanning strategy at different heat input levels: (a) Engineering stress-strain curves illustrating the tensile behavior across varying heat inputs. (b) Micro-hardness profiles measured along the build direction, showing the effect of heat input on hardness distribution.

Table 5.7: Comparison of the tensile properties of the printed samples at varying heat input levels.

Heat input (J/mm)	Location	0.2% YS (MPa)	UTS (MPa)	Elongation (%)
232 J/mm	Top	1098±26	1221±31	2.6±0.2
	Middle	988±24	1095±28	1.5±0.1
	Bottom	903±22	1093±27	2±0.2
	Top	1075±25	1090±26	1.14±0.1

310 J/mm	Middle	951±23	1285±34	1.12±0.1
	Bottom	900±21	1245±32	1.03±0.1
	Top	860±20	1211±29	2±0.2
465 J/mm	Middle	819±11	1221±30	2±0.2
	Bottom	843±7	1186±38	2.15±0.2

Figure 5.35 presents the fracture morphologies of the printed walls at various locations, scanning strategies, and heat input levels, providing critical insights into how these factors influence the mechanical performance and fracture behavior of the material. For the uni-directional tensile samples, the fracture surfaces exhibit a mixed mode of failure, characterized by tearing ridges, quasi-cleavage facets, and dimples, as shown in Figure 5.35 (a-c). The presence of intergranular fractures, highlighted by blue arrows, indicates the contribution of residual stress and thermal gradients resulting from the uni-directional scanning strategy. Additionally, the heterogeneous orientations of martensitic laths create distinct river patterns on the fracture surfaces, further reflecting the anisotropic nature of the microstructure and stress distribution. In contrast, the bi-directional scanning strategy demonstrates a significant improvement in fracture behavior. At the bottom location with a lower heat input of 245 J/mm, the fracture surfaces display fine equiaxed dimples (Figure 5.35 d), signifying ductile failure. This correlates with the uniform heat distribution and reduced residual stress enabled by the bi-directional scanning strategy, which promotes better deformation and energy absorption during tensile loading. However, at a higher heat input of 310 J/mm in the top region, the fracture mode transitions to quasi-cleavage, characterized by the presence of cleavage facets and tearing ridges interspersed with small dimples (Figure 5.35 e). This transition is driven by slower cooling rates at upper layers, which result in grain coarsening and an increase in residual stress. Interestingly, at elevated heat inputs of 310 J/mm and 465 J/mm in the bottom region, the fractured surfaces still display predominantly ductile features, such as equiaxed dimples (Figure 5.35 f-g). This behavior is linked to the lower magnitude of tensile residual stress near the substrate, as observed in numerical simulations, which contributes to improved ductility in these regions.

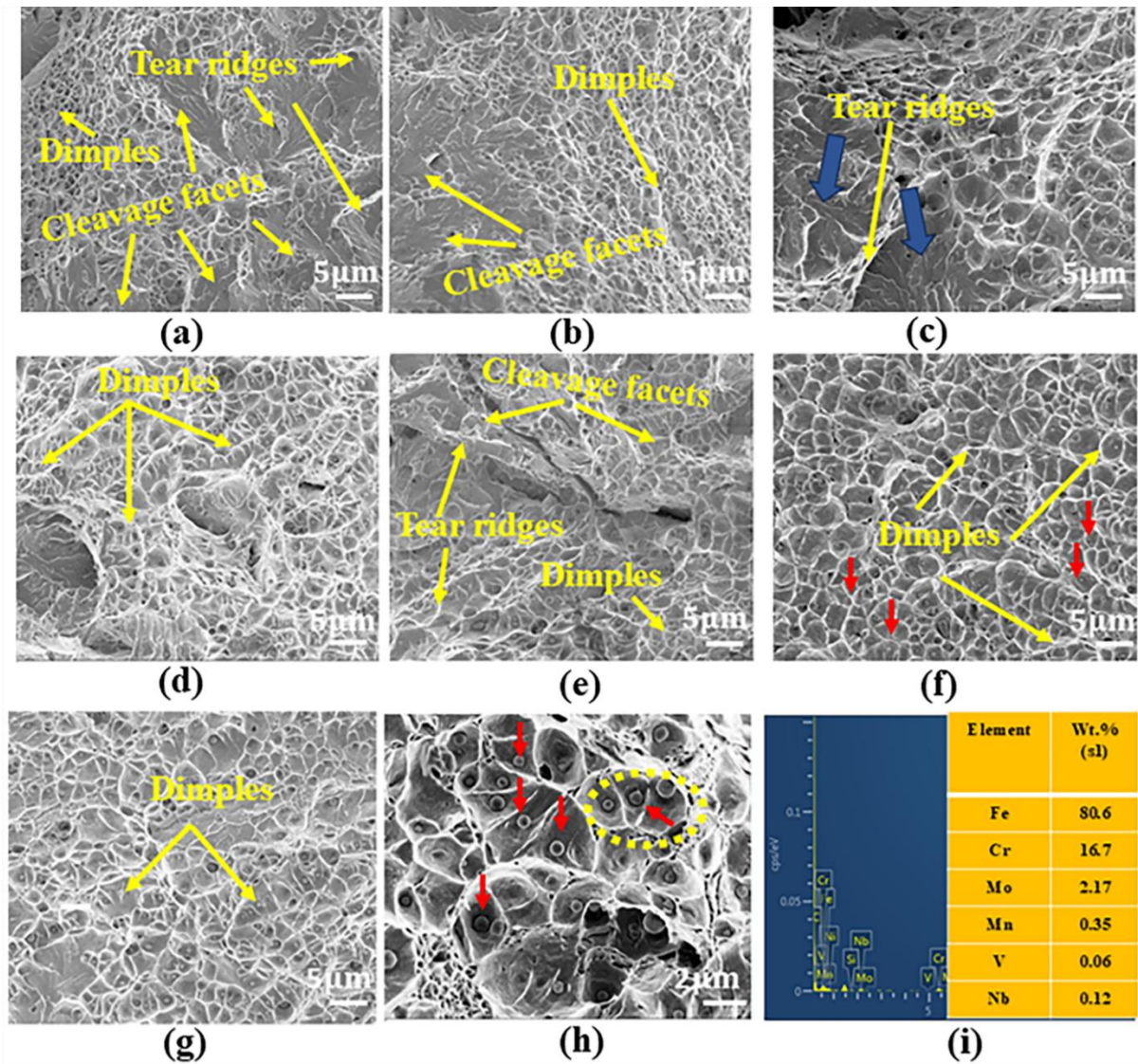


Figure 5.35: Morphology of the fractured tensile samples extracted from different locations (top, middle, and bottom) along the build direction: (a–f) Comparison of fracture morphologies in uni-directional and bi-directional printed samples at a heat input of 310 J/mm, highlighting differences in fracture modes. (g–i) Morphology of fractured samples printed at a high heat input level, showing the effect of heat input on fracture characteristics.

Higher magnification analysis of the fracture surfaces (Figure 5.35 h) reveals the presence of numerous precipitates embedded within large dimples, marked by red arrows and yellow dashed circles. These precipitates, identified as MX and $M_{23}C_6$ carbides through EDS analysis and thermodynamic modelling [197], play a critical role in dictating fracture behavior. During

tensile testing, microcracks nucleate at these precipitates and propagate into larger deformation zone, enhancing the ductility of the material compared to quasi-cleavage failure modes. Larger dimples are associated with $M_{23}C_6$ carbides, which coarsen along grain boundaries during deposition. This behavior underscores the impact of precipitate morphology and distribution on mechanical properties and fractured mechanisms.

Overall, the findings highlight that fracture behavior transitions from quasi-cleavage to ductile failure as the scanning strategy changes from uni-directional to bi-directional and as the distance from the substrate decreases. The bi-directional scanning strategy's ability to alternate heat input across layers not only reduces residual stress and thermal gradients but also enhances microstructural uniformity and mechanical stability. These observations reinforce the role of deposition strategy and heat input modulation in tailoring the fracture performance of additively manufactured components, making the bi-directional approach more suitable for applications requiring improved properties and reliability.

5.5 Designing and development of advanced scan pattern

Arc-based DED of 9Cr–1Mo steel has emerged as a promising route for fabricating structural components for AUSC power plants, yet the control of martensitic transformation and residual stress remains a major challenge since both directly govern long-term creep resistance and the onset of Type IV failure. Conventional unidirectional scanning strategies impose steep thermal gradients, which in turn non-uniform residual stress distribution, and degradation of service performance. To address these limitations, the concept of scan path engineering has gained attention. Wherein the modulation of heat flow is exploited to actively influence transformation kinetics, refine martensitic lath morphology, and redistribute tensile and compressive stresses across the deposited structure. The integration of dilatometry, EBSD, and XRD-based residual stress measurements has already revealed that non-equilibrium thermal cycles inherent to DED can be harnessed to tune transformation-induced strain and suppress localized stress accumulation. Complementing these experiments, FE-based TMM models, strengthened by incorporation of dilatometric strain data, enable predictive assessment of coupled temperature, stress, and phase transformation effects, while emerging AI frameworks such as TCN provide fast surrogates for mapping transient thermal histories to dilatometric response. Within this framework, the design of advanced scanning strategies

ranging from spiral-in/out, inclined, circular, S and mixed patterns offers a powerful means to redistribute heat, regulate local martensitic transformation behavior, and minimize tensile residual stress, thereby ensuring structural integrity and extending the high-temperature durability of 9Cr–1Mo steel components produced via arc-DED.

5.5.1 Evaluation of temperature history

The simulated 3D temperature profiles illustrate the thermal fields associated with two scanning strategies: the complete longitudinal deposition path and the mid-section of the circular pattern (Figure 5.36 a and b). The temperature ranges from 761°C to 945 °C corresponds to the critical austenitization window, bounded by A_{c1} and A_{c3} , within which the transformation from tempered martensite to austenite occurs. The solidus–liquidus gap in 9Cr–1Mo steel, approximately 80°C is shown in red to indicate mushy region. This zone reflects the transition between the onset and completion of melting. The temperature ranges from the minimum value (T_{min}) up to 577°C also encompasses the martensitic transformation domain during cooling. The mushy zone is observed to be broader at the trailing edge of the melt pool and comparatively narrower at the leading edge, indicating directional solidification. The molten pool, represented by a grey ellipsoidal region, delineates the high-temperature liquid phase during active deposition.

Thermal histories associated with six distinct scanning strategies demonstrate significant variation in peak temperature, heating rate, and cooling behavior during DED of 9Cr–1Mo steel (Figure 5.36). Experimentally measured time-temperature profiles (using thermocouples) are compared with finite element simulations extracted from the same spatial location of the substrate. The longitudinal scanning strategy exhibits a rapid thermal rise, reaching a peak of approximately 1085°C at 22 s, followed by sharp cooling to below 300°C within 20 s (Figure 5.36 c). The simulated profile closely reproduced this thermal trajectory, with a maximum deviation of less than 20 °C, confirming accurate modeling of directional heat conduction and steep thermal gradients. The spiral configuration, where the heat input converges toward the center, the thermal profile showed a gradual temperature rise, reaching a peak of 1058 °C at approximately 25 s, followed by an extended dwell at elevated temperature (Figure 5.36 d). The simulated curve effectively captured the delayed peak and thermal accumulation, deviating by less than 15°C. Conversely, the inclined scanning pattern resulted in the most

uniform thermal distribution among all strategies. The peak temperature reached 1042°C, accompanied by a stable high-temperature plateau (Figure 5.36 e). Simulated results show reasonable correlation, with a maximum discrepancy of less than 10°C, underscoring the robustness of the model in capturing multidirectional heat flow and thermal dispersion. In contrast, the circular strategy, involving concentric heat input, led to the most severe thermal accumulation, with a peak of 1092°C and a slow cooling cycle caused by repetitive reheating of the central region (Figure 5.36 f). Though the simulation slightly underestimated the peak by approximately 25°C, it effectively reproduced the prolonged thermal retention, validating the model's suitability for scenarios involving complex thermal overlap. Across all scanning strategies, the root-mean-square error (RMSE) between simulated and experimental profiles ranged from 12 to 25 °C, indicating a strong correlation between the modelled and observed thermal behaviors. These validated profiles establish a reliable foundation for subsequent thermo-metallurgical and phase transformation modelling, thereby facilitating predictive control over microstructural evolution in DED fabrication of ferritic–martensitic steels.

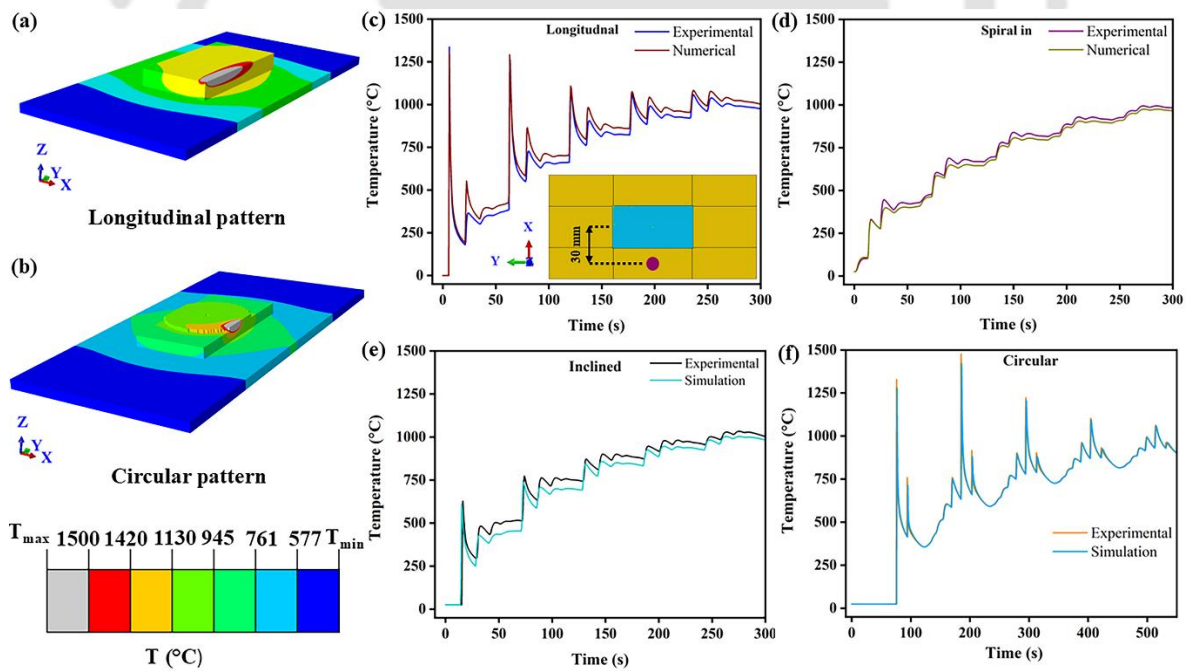


Figure 5.36: (a, b) Simulated thermal profile for longitudinal and circular patterns; (c, d, e, f) comparison of experimentally measured and simulated transient temperature profiles at a distance of 30 mm from the centerline of the deposit.

5.5.2 Phase transformation kinetics

The dilatometric strain–temperature profile corresponding to the longitudinal scanning strategy is employed to extract critical transformation parameters (Figure 5.37 a). While deposition of material, phase transformations are primarily reflected through distinct volumetric changes of the evolving phases, and these changes exhibit a linear correlation with the corresponding phase fractions. During heating cycle the critical austenite transformation temperatures $A_{C1} = 864\text{ }^{\circ}\text{C}$. Between A_{C1} and $A_{C3} = 907\text{ }^{\circ}\text{C}$, the curve shows a net contraction despite rising temperature, evidencing progressive $\alpha'/\alpha \rightarrow \gamma$ transformation; over this interval the effective strain–temperature slope is $2.3 \times 10^{-4}\text{ }^{\circ}\text{C}^{-1}$. Figure 5.37 b depicts the measured thermal expansion curve along with the corresponding transformation fraction during cooling. The onset ($M_s = 397^{\circ}\text{C}$) and competition ($M_f = 300^{\circ}\text{C}$) of the martensitic transformation are determined using the double-tangent method.

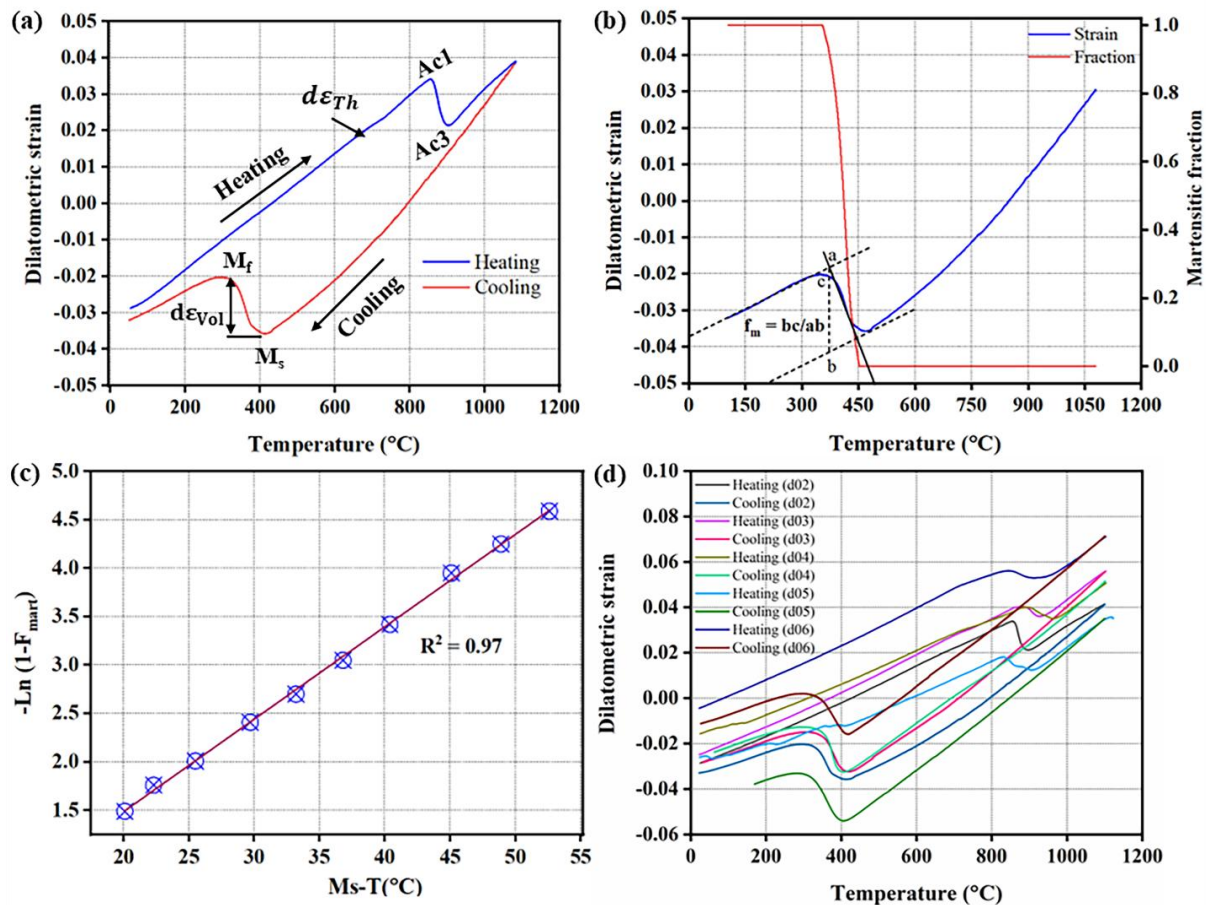


Figure 5.37: Dilatometric study and phase transformation behavior: (a) Dilatometric strain during heating and cooling cycles at constant rate for longitudinal scan, marking with A_{c1} , A_{c3} , M_s , M_f , thermal strain and volumetric strains; (b) evolution of martensitic fraction for longitudinal scan; (c) linearly fitted curve for the evaluation of martensitic transformation constant (k); and (d) dilatometric strain responses for five additional scan strategies.

Volumetric changes associated with the complete martensitic transformation corresponds to a strain of 1.49×10^{-2} . The evolution of the martensitic transformation fraction during cooling was derived using the lever rule applied to the dilatometric curve. The martensitic transformation constant k in the Koistinen–Marburger (KM) equation is determined by curve fitting of the experimental data, as shown in Figure 5.37b. Linearly fitted curve between $-\ln(1 - F_{mart})$ and $(M_{start} - T)$ holds only over a narrow temperature interval where martensitic transformation occurs (Figure 5.37c). Therefore, a sliding window (i.e., small subsets of adjacent data points) is used across the valid region (from M_f to M_s with $F_{mart} \in [0, 0.98]$) to fit multiple straight lines. The best-fitting segment is selected by checking higher R^2 value. From this method, the best linear region is determined with $k = 0.0796 \sim 0.08$ and coefficient of determination ($R^2 = 0.9652$). Dilatometric responses for remaining scan patterns are illustrated in Figure 5.37d. For the computation of residual stress, transformation temperatures and slope of each scan pattern during heating and cooling cycles from dilatometric responses correspond to each scan are incorporated in numerical simulations.

XRD analysis is conducted on samples fabricated with different scanning strategies to evaluate the phase constitution and crystallographic behavior of the deposited 9Cr-1Mo steel. The XRD patterns across all strategies revealed three principal diffraction peaks corresponding to the $\{110\}$, $\{200\}$, and $\{211\}$ planes of the α -ferrite phase with a BCC crystal structure, occurring at approximately 44.6° , 64.8° , and 82.3° , respectively (Figure 5.38). These reflections confirm the predominance of BCC ferrite in the microstructure, a characteristic feature of ferritic-martensitic steels subjected to rapid thermal cycles during DED. Although the XRD results consistently indicate the presence of the BCC α -ferrite phase, no distinct martensitic peaks are discernible. This apparent absence of martensitic signatures can be ascribed to the inherent crystallographic similarity between the α -ferrite and martensite structures in 9Cr-1Mo steel. Given that the martensite formed in this alloy exhibits a BCC

structure with a tetragonality ratio (c/a) deviating only marginally from unity, typically on the order of 10^{-4} to 10^{-5} [193]. As a result, martensite cannot be resolved as a distinct phase but instead contributes to the overall BCC diffraction pattern, rendering the XRD profile representative of a combined ferritic–martensitic microstructure.

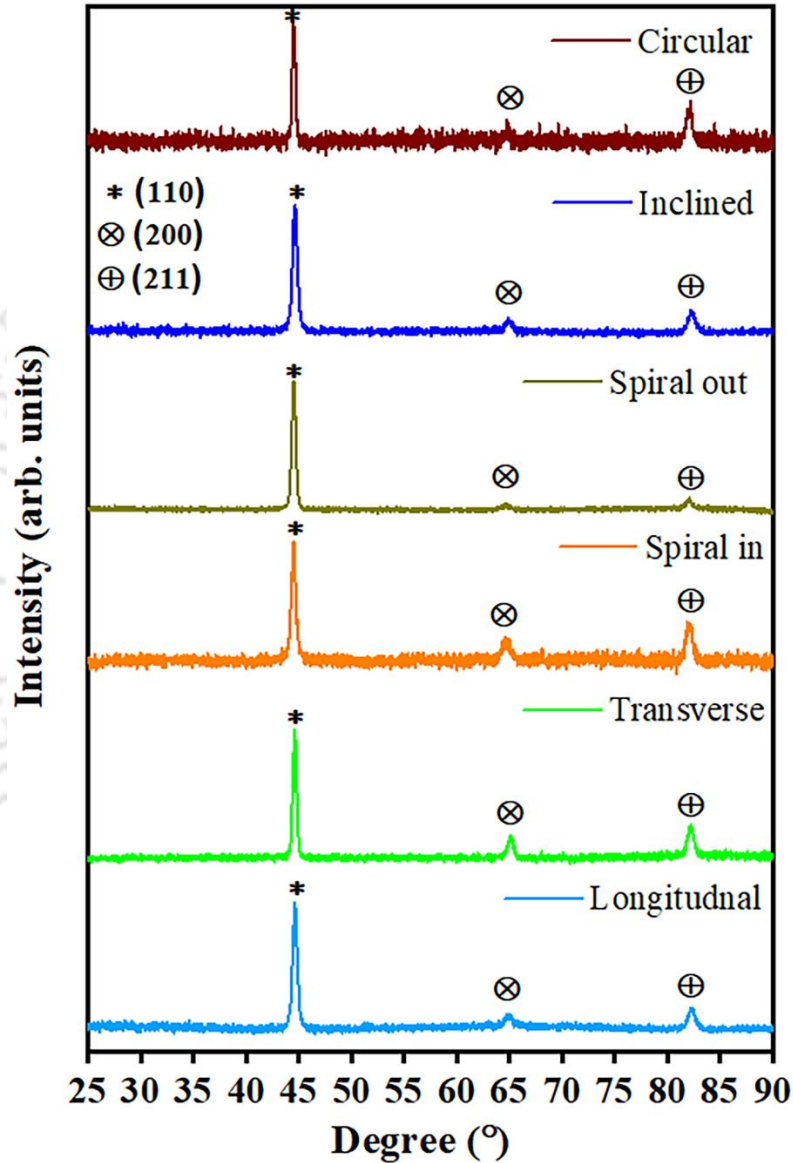


Figure 5.38: XRD profiles showing intensity versus 2θ for 9Cr–1Mo steel samples fabricated using different scanning strategies.

To elucidate sub-grain scale transformations beyond XRD detection, EBSD-based IQ and IPF maps are employed to track lattice integrity, strain content, and crystallographic texture

under different scanning strategies. In the longitudinal strategy, consistently high IQ values indicate refined martensitic laths with high dislocation density and minimal δ -ferrite, correlating with IPF maps that show a dominant $\{001\}$ orientation along the build direction, thereby generating strong anisotropy and elevated residual stress aligned with the wall axis (Figure 5.39 a₁ and b₁). In contrast, the spiral-in pattern, characterized by heat accumulation at the core, produces reduced IQ values and visible δ -ferrite regions due to repeated reheating and tempering; this is reflected in the IPF maps by redistribution of orientations toward a mixed $\{001\}/\{111\}$ texture, enhancing ductility but compromising homogeneity (Figure 5.39 a₂ and b₂). The spiral-out strategy results in relatively higher IQ quality at the center with gradual degradation toward the edges, consistent with stable martensitic transformation in the core and partial tempering at the periphery; IPF maps corroborate this with fine laths preferentially aligned along $\{001\}$ and $\{101\}$, yielding balanced residual stress and limited δ -ferrite (Figure 5.40 a₃ and b₃). In the inclined strategy, diagonal heat flow disperses thermal gradients, giving rise to spatially heterogeneous IQ regions and a broad spread of $\{001\}$, $\{101\}$, and $\{111\}$ orientations in IPF maps; this orientation diversity reduces overall residual stress while δ -ferrite remains minimal and randomly distributed (Figure 5.39 a₄ and b₄). Finally, the circular strategy, dominated by concentric reheating, exhibits extensive IQ degradation and widespread δ -ferrite at the core, matched by a strong $\{111\}$ orientation in IPF maps that favours slip compliance but undermines crystallographic uniformity (Figure 5.39 a₅ and b₅). Collectively, these results establish that each scanning pattern imposes a distinct thermal history that dictates martensitic refinement, δ -ferrite evolution, residual stress state, and texture, thereby linking process strategy directly to microstructural and mechanical performance.

Building upon the crystallographic orientation data from the IPF maps, the Grain Orientation Spread (GOS) analysis provides a quantitative assessment of intragranular misorientation and serves as a sensitive indicator of residual stress and lattice distortion within individual grains [198,199]. The GOS value for a given grain i is calculated as:

$$GOS(i) = \frac{1}{J(i)} \sum_{j=1}^{J(i)} x_{ij} \quad (1)$$

where x_{ij} depicts the misorientation angle between pixel j and the mean orientation of grain i , and $J(i)$ is the number of pixels constituting that grain. Different scan patterns are found to

significantly influence lattice distortion, residual stress, and texture evolution in 9Cr-1Mo steel deposits. Longitudinal, spiral-out, and circular patterns produced higher GOS values (Figure 5.39 c₁, c₃, c₅), indicative of severe lattice distortion and retained transformation stresses due to directional heat flow or repetitive thermal cycling, with the circular path showing the strongest central stress concentration despite limited δ -ferrite formation. In contrast, inclined and in-out strategies yielded lower GOS values (Figure 5.39 c₂, c₄), reflecting improved thermal distribution and stress relaxation. EBSD phase maps (Figure 5.39 d₁–d₅) confirmed a predominantly martensitic microstructure (>99% BCC/BCT) in all cases, as inter-pass temperatures remained below M_s , ensuring near-complete austenite-to-martensite transformation while suppressing retained austenite and δ -ferrite. Pole figure analysis of the $\{001\}$ BCT plane (Figure 5.39 e₁–e₅) revealed the strongest texture in the longitudinal strategy (9.2 m.r.d.), moderately strong orientations in spiral-in/out (8.9, 8.6 m.r.d.), a more diffuse alignment in the inclined scan (8.1 m.r.d.), and the weakest texture in the circular pattern (7.8 m.r.d.), consistent with the corresponding residual stress distributions.

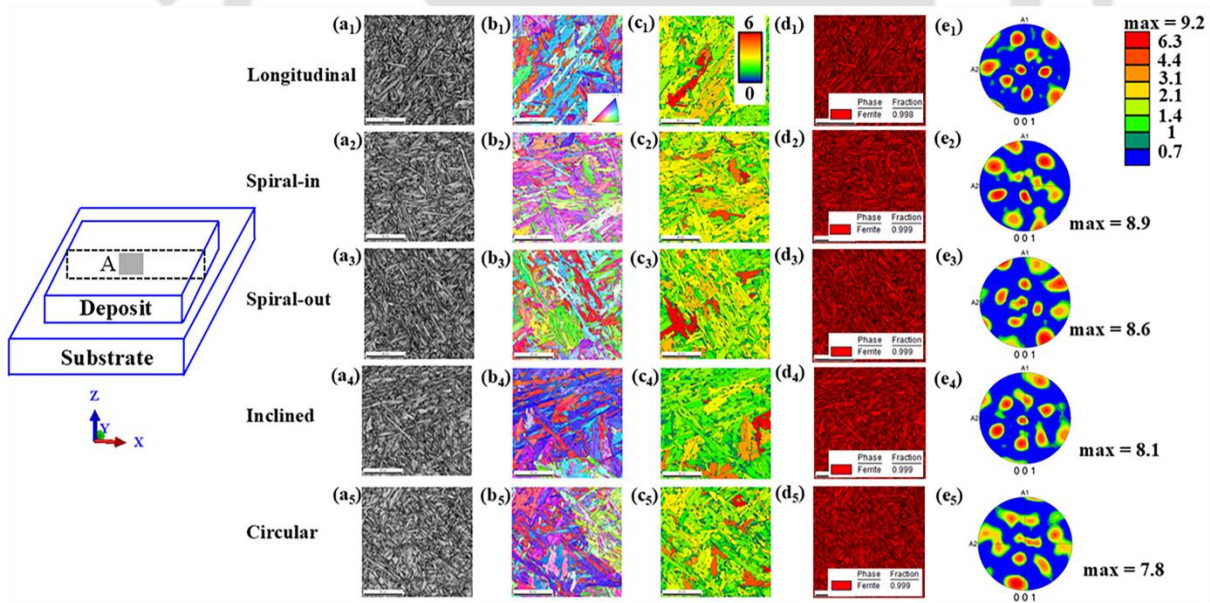


Figure 5.39: EBSD-based microstructural characterization of different scanning strategies: (a₁–a₅) IQ maps; (b₁–b₅) IPF maps showing crystallographic orientation with respect to the build direction; (c₁–c₅) GOS maps highlighting local misorientation and internal strain; (d₁–d₅) Phase maps identifying the distribution of phases present; and (e₁–e₅) pole figures reflecting texture evolution for each scan strategy.

5.5.3 Computation of residual stress including the effect of phase transformation kinetics

The spatial–temporal distribution of von Mises residual stress in CMT-DED-processed 9Cr–1Mo steel is intricately governed by thermal gradients and crystallographic evolution imposed by distinct scanning strategies. In the longitudinal scan, where heat is directed along the build length, residual stress peaks at $S_{\max} \approx 535.2$ MPa near the clamping zone due to sharp directional cooling and constrained shrinkage (Figure 5.40a). The lowest martensitic fraction ($F_m \approx 0.88$) indicates incomplete transformation, which limits the microstructural ability to accommodate thermal contraction. EBSD IPF maps show a dominant $\{001\}$ texture aligned with the build direction, while elevated GOS values indicate significant lattice distortion. In the transverse scan, stress reduces slightly ($S_{\max} \approx 516.7$ MPa) due to enhanced lateral heat flow (Figure 5.40b). This supports a higher martensitic fraction ($F_m \approx 0.97$), resulting in more balanced microstructure formation and improved thermal compatibility. GOS values are moderate, consistent with refined lath packets and improved plasticity. The spiral-in strategy introduces severe central thermal accumulation, producing an anomalously high residual stress peak ($S_{\max} \approx 5071.1$ MPa) likely due to numerical singularity (Figure 5.40c). Nonetheless, this signifies intense localized contraction where thermal cycles overlap. The martensitic fraction remains high ($F_m \approx 0.99$), with moderate GOS values, explain the limited effectiveness of transformation in mitigating residual stress.

In the spiral-out strategy, which begins at the center and proceeds outward, thermal gradients are better managed. This results in a maximum stress of 515.7 MPa and minimal stress of 2.8 MPa (Figure 5.40d). A complete martensitic transformation ($F_m = 1.0$) enables more efficient stress relief. GOS values confirm reduced lattice misorientation in the central region. The microstructural balance between phase evolution and spatial heat flow enables favorable stress accommodation. The inclined scanning strategy, which introduces diagonal energy flow, yields the most uniform residual stress distribution ($S_{\max} \approx 521.7$ MPa, $S_{\min} \approx 2.1$ MPa) across the build (Figure 5.40e). It achieves complete martensitic transformation ($F_m = 1.0$), promoting high microstructural stability, while the lowest GOS values point to minimal internal misorientation. Finally, the circular scan results in the highest actual residual stress ($S_{\max} \approx 620$ MPa), particularly at the clamping edge and outer periphery (Figure 5.40f). Concentric thermal cycling amplifies cumulative heat retention and triaxial contraction. While the martensitic fraction remains high ($F_m \approx 0.98$), while favorable for slip, are mechanically

compliant and contribute to reduced load-bearing capability. The GOS is highest among all strategies, confirming extensive lattice distortion. Consequently, despite the near-complete martensitic transformation, poor crystallographic alignment and δ -ferrite presence limit the effectiveness of this strategy in stress relief.

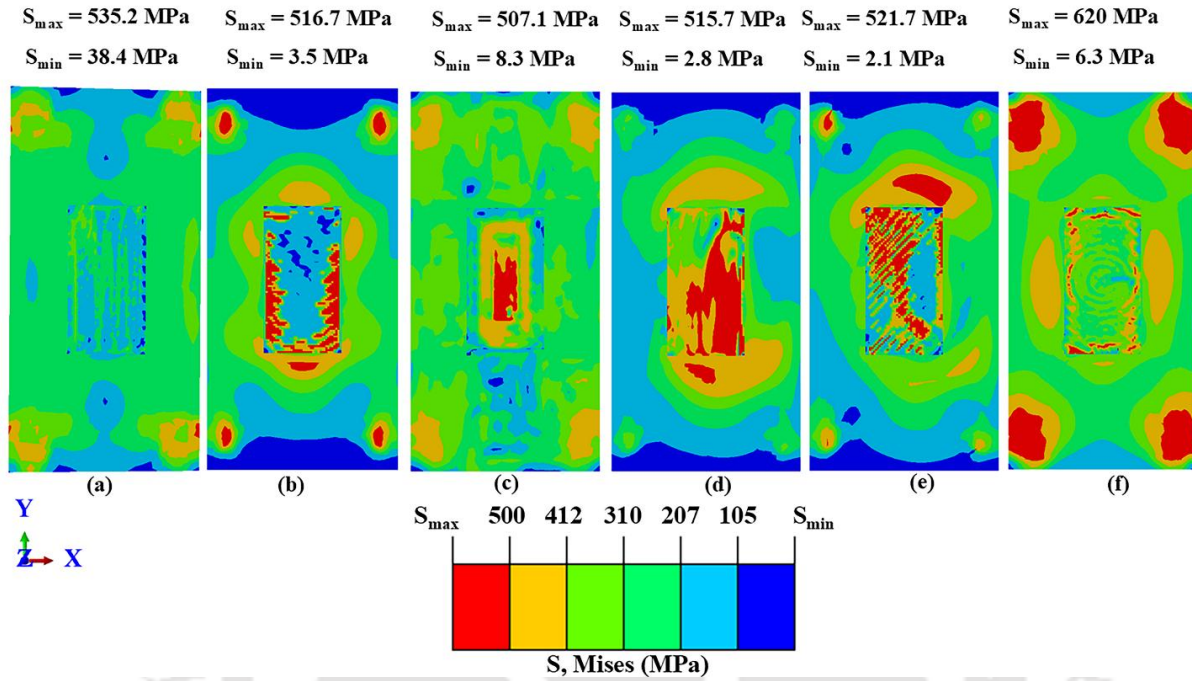


Figure 5.40: Von Mises residual stress fields in 9Cr-1Mo steel components fabricated using different scanning strategies.

A comparative analysis of numerically predicted and experimentally validated residual stress magnitudes for different scanning strategies provides critical insight into the underlying thermo-metallurgical mechanisms along y'-y' axis of printed part (Figure 5.41 a-c). The longitudinal scan, characterized by unidirectional heat input and sharp thermal gradients, exhibited the lowest kinetic-mechanical index ($K_m = 0.67 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$) (Figure 5.41 d). The transformation-induced strain (-0.0097), suggesting dominant tensile mismatch or suppressed expansion due to constrained cooling, which translated into a high residual stress of 543.5 MPa (Figure 5.41 a). In contrast, the transverse scan, with lateral heat conduction, enabled enhanced phase transformation dynamics producing a strain of 0.01475 and a moderate K_m of $1.13 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$. This improved the stress accommodation, resulting in a reduced residual

stress of 465.18 MPa (Figure 5.41 a and d). The spiral-in pattern supported a gradual and uniform heat flow toward the center, promoting a martensitic fraction of ~ 0.99 and strain of 0.01508, leading to a higher K_m ($1.17 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$) and the lowest residual (296.11 MPa) (Figure 5.41 b and d). Its inward geometry aids uniform cooling and facilitates efficient martensitic expansion. Similarly, the spiral-out scan showed complete martensitic transformation, with K_m of $1.52 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$, enabling substantial plastic accommodation and limiting residual stress to 349.05 MPa, despite some heat retention near the center. The inclined scan, which combines directional heating at 45° , achieved the highest transformation strain (0.02064) and K_m ($1.62 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$), indicating maximal transformation plasticity; however, residual stress remained moderate (468.66 MPa), likely due to complex stress interactions and localized incompatibility in phase expansion (Figure 5.41 c and d). Finally, the circular scan, though it showed a relatively high strain (0.01549) and favorable transformation kinetics ($F_m \approx 0.98$), resulted in the highest residual stress (656.46 MPa) due to concentric heat accumulation and triaxial constraint effects.

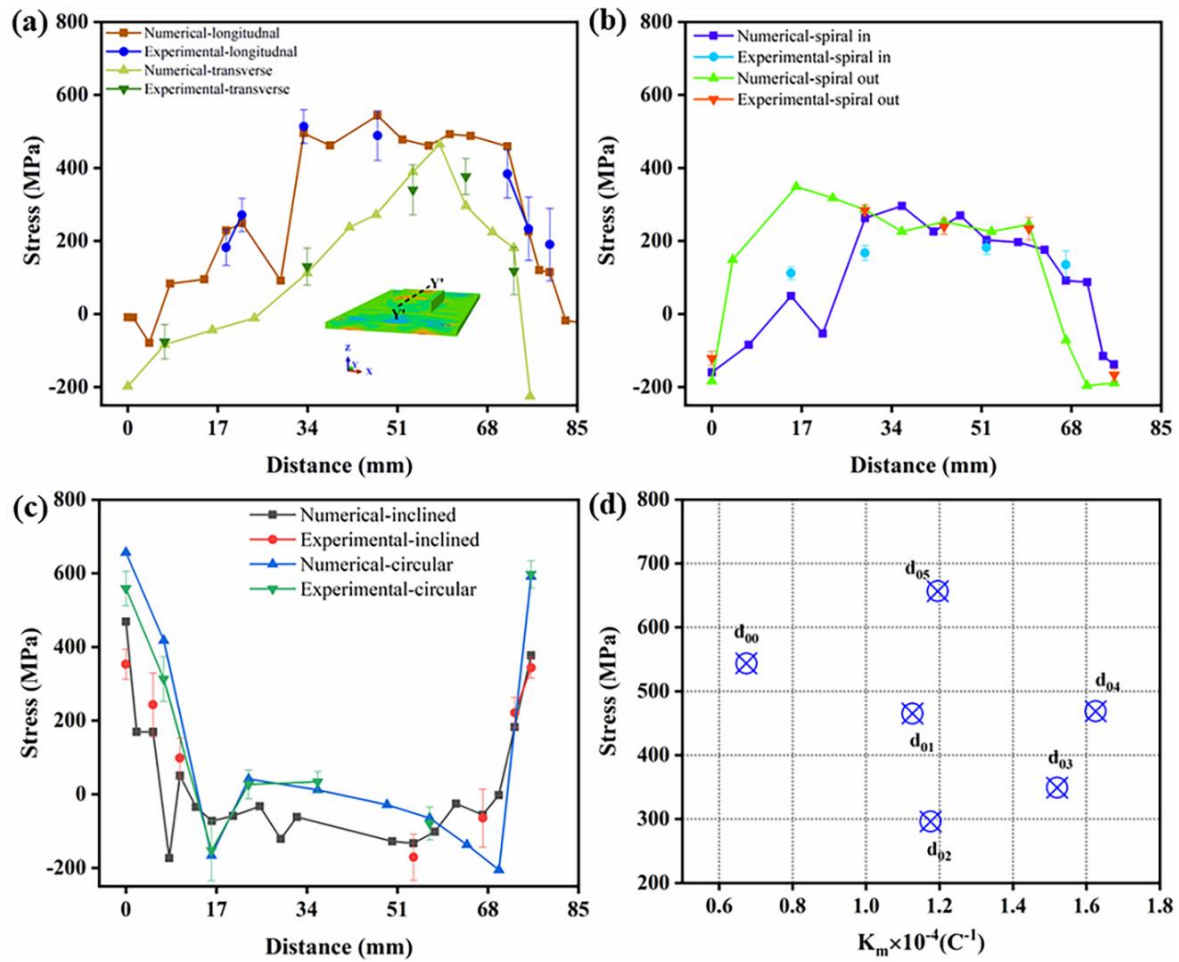


Figure 5.41: Numerical and experimental evaluation of longitudinal residual stress component (S_{11}) in 9Cr-1Mo steel components fabricated using different scanning strategies: longitudinal, transverse, spiral-in, spiral-out, inclined, and circular (a–c). Experimental data are shown with standard deviation error bars, while numerical predictions incorporate spatially resolved thermal gradients and phase transformation kinetics. Subfigure (d) presents the correlation between maximum longitudinal residual stress and K_m .

5.5.4 Mechanical characterization of printed samples

The tensile behavior of 9Cr-1Mo steel fabricated DED process demonstrates significant deviation in mechanical performance from the conventionally manufactured and tempered base material, primarily due to rapid solidification, directional heat input, and transformation-induced microstructural evolution (Figure 5.42 a and b). Base material, characterized by a tempered martensitic microstructure formed under near-equilibrium conditions, exhibits a UTS

of 751.7 MPa, YS of 478 MPa, and elongation of 17.8%, reflecting a balanced strength–ductility profile supported by low dislocation density and homogeneous tempering. In contrast, the longitudinal scan promotes significant martensitic transformation with lower K_m suggest suppressed transformation kinetics (Figure 5.42 c). These conditions result in a refined lath martensitic structure with elevated dislocation density, contributing to high UTS (1275.5 MPa) and YS (1075.4 MPa). However, the unrelieved tensile residual stresses aligned along the scan direction constrain plastic deformation, reducing elongation to 13.6%. While Transverse scans, by reorienting the scan path perpendicular to the build direction, facilitates lateral heat dissipation and more uniform interlayer reheating. This promotes a higher martensitic fraction accompanied by an increased K_m . These thermal and kinetic advantages improve stress redistribution through enhanced martensitic plasticity and reduced residual stress anisotropy. As a result, the transverse scan achieves a high UTS of 1341.1 MPa, YS of 1074.3 MPa, and a moderate elongation of 16.3%.

Radially symmetric strategies like in-out and out-in (spiral) introduce divergent thermal field distributions. The in-out pattern, with heat progressing inward, leads to thermal accumulation at the center, driving intense cooling rates and promoting near-complete martensitic transformation. These conditions yield high UTS (1516.5 MPa) and YS (1125.3 MPa), supported by elevated dislocation density due to TRIP. However, localized stress concentration at the center constrains elongation (18.6%), despite the strength gain. Conversely, the out-in pattern dissipates heat outward, creating a broader melt pool and reduced stress at the center. With complete martensitic transformation and the highest K_m among spiral strategies, this scan achieves UTS (1387.3 MPa) and YS (1066.3 MPa) with elongation of 18.1%, highlighting the trade-off between stress relief and retained strength. The inclined scan, delivering heat at a 45° angle to both axes, generates multidirectional thermal gradients that foster uniform phase transformation and efficient strain accommodation. With the highest martensitic transformation and maximum K_m , this pattern leads to the highest UTS (1587.0 MPa) and YS (1186.8 MPa). The distributed dislocation structure and minimal thermal anisotropy facilitate effective residual stress mitigation, enabling excellent elongation (19.1%) making it the most mechanically robust strategy. In contrast, the circular scan, despite its geometric symmetry, causes concentric heat accumulation that disrupts uniform transformation, triaxial stress build-up at the center impedes full plastic accommodation. As a

result, while UTS (1398.6 MPa) and YS (1040.8 MPa) remain strong, elongation is limited to 12.9%, the lowest among all DED variants.

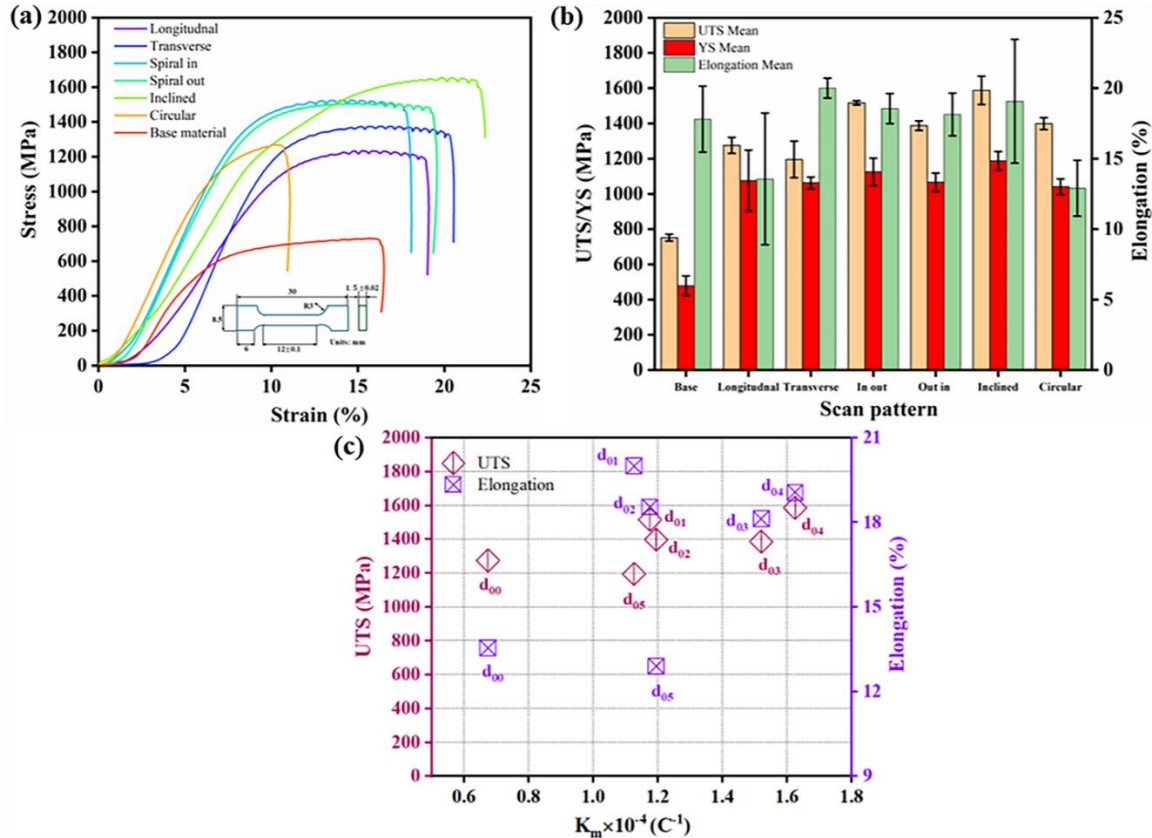


Figure 5.42: Influence of scanning strategies on tensile behavior of directed energy deposited 9Cr–1Mo steel (a, b); and (c) correlation of UTS and elongation with K_m .

The microhardness distribution in DED of 9Cr–1Mo steel components demonstrates a strong correlation with K_m , F_m , and dislocation density parameters fundamentally governed by the thermal history induced by each scanning strategy (Figure 5.43). The longitudinal scan yields a low K_m and an incomplete martensitic transformation ($F_m \approx 0.88$). The constrained volumetric change and reduced transformation-induced plastic strain dislocation accumulation, resulting in a moderate microhardness of 466.9 HV, despite the presence of martensite (Figure 5.43 a and d). The residual stress is high due to rapid cooling and insufficient stress accommodation. In contrast, the transverse scan, associated with a higher K_m and martensitic fraction of ~ 0.97 , promotes better thermal redistribution. However, the broader

heat-affected zone and moderated cooling rates reduce dislocation density slightly, producing the lowest microhardness of 450.8 HV among all strategies, despite a higher transformation fraction. This suggests that microhardness is not only governed by F_m but also by how transformation strain is accommodated via dislocation storage.

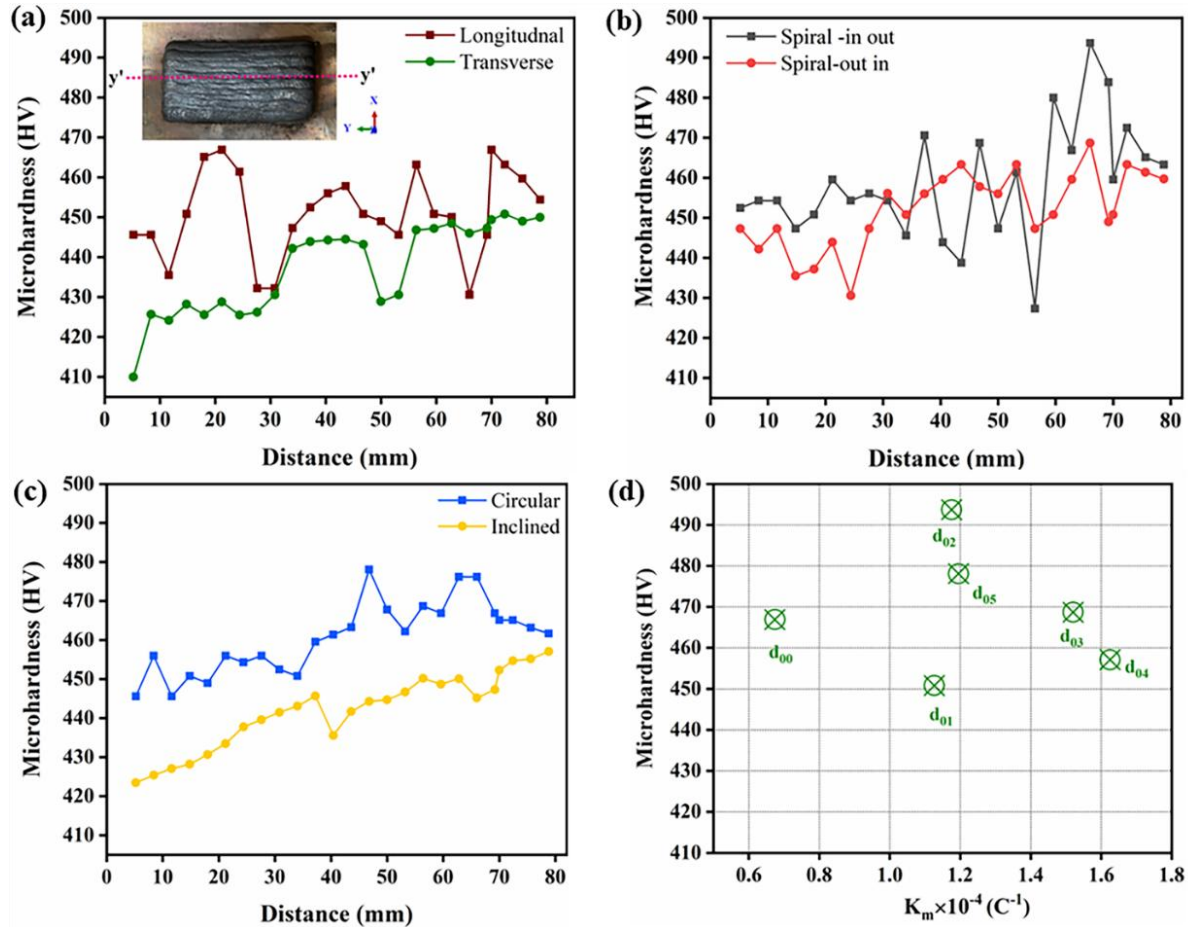


Figure 5.43: Microhardness variation of 9Cr-1Mo steel fabricated using different scanning strategies in DED (a, b, c) and (d) scatter plot of maximum microhardness versus K_m .

The spiral-in scan shows the most favourable combination of parameters: a high K_m , nearly complete martensitic transformation ($F_m \approx 0.99$), and sharp inward cooling that traps high dislocation density. This results in the maximum microhardness of 493.7 HV, reflecting the synergistic effect of complete transformation and constrained strain accommodation due to radial heat concentration (Figure 5.44 b and d). Similarly, the spiral-out scan achieves full martensitic transformation and a higher K_m , but due to outward heat flow, the thermal gradients

are less steep, and some strain recovery may occur. Thus, the microhardness drops slightly to 468.7 HV, indicating partial dislocation rearrangement and reduced residual strain retention. The inclined scan, despite achieving the highest K_m and full martensitic transformation, results in a microhardness of 457.1 HV. This is likely due to more isotropic heat flow, allowing for dynamic recovery or dislocation annihilation, which offsets the hardening from martensitic formation (Figure 5.44 c and d). Lastly, the circular scan delivers a well-balanced thermal profile with high F_m (~ 0.98), and substantial dislocation entrapment due to symmetrical heat input. It results in a high microhardness of 478.1 HV, although triaxial stress development near the centre introduces complex local softening and hardening zones.

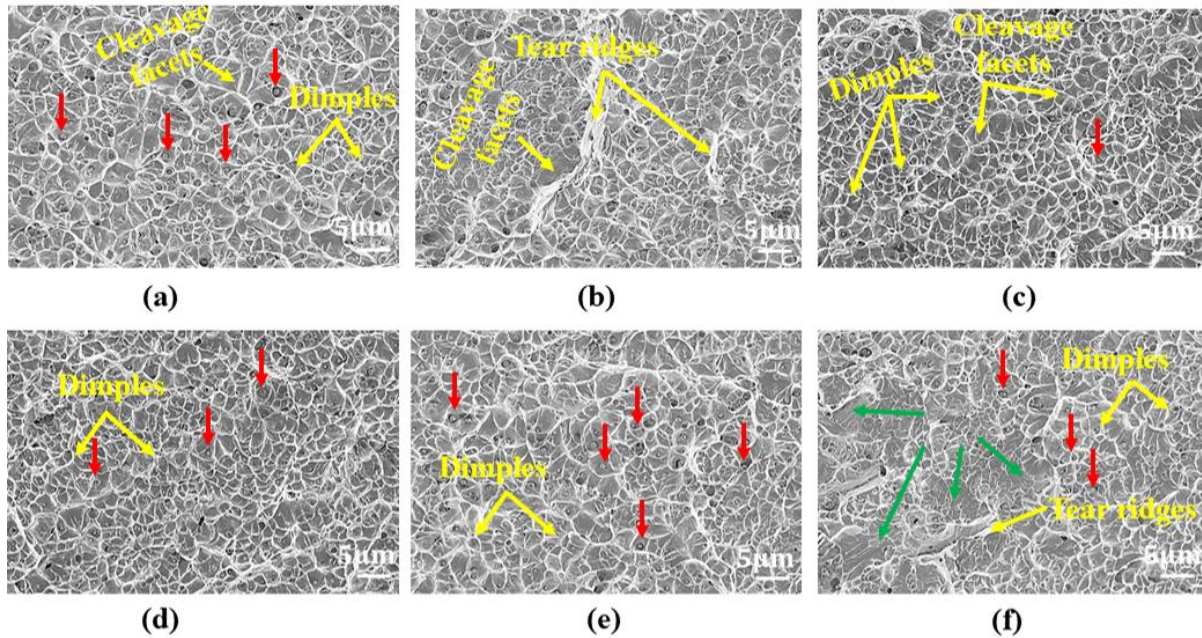


Figure 5.44: SEM micrographs of fracture surfaces for tensile-tested 9Cr–1Mo steel samples fabricated via CMT-based DED under varying scanning strategies (a, b, c, d and e).

Fractographic evaluation of tensile-tested samples fabricated via CMT-DED under different scanning strategies reveals a strong correlation between fracture morphology, martensitic transformation behavior, and residual stress evolution. The longitudinal scans, associated with the lowest martensitic fraction, exhibit dominant quasi-cleavage fracture features with limited ductile dimpling (Figure 5.44 a). This brittle nature is attributed to poor transformation-induced accommodation of thermal contraction and low transformation

kinetics, both of which promote elevated residual stress and early crack initiation. Conversely, the transverse scan, with improved martensitic fraction and moderately enhanced transformation kinetics, transitions toward a mixed-mode fracture. The increased presence of ductile dimples suggests enhanced energy dissipation capacity due to refined lath morphology and better dislocation activity (Figure 5.44 b). In the spiral-in and spiral-out strategies, near-complete or complete martensitic transformation is observed, accompanied by elevated transformation kinetics. These conditions foster deeper and more uniformly distributed dimples, indicating improved plasticity and delayed crack propagation. However, subtle differences exist between them spiral-in shows more pronounced central softening due to thermal accumulation, while spiral-out maintains better structural integrity at the core with slightly reduced peripheral ductility (Figure 5.44 c and d). The inclined scan pattern stands out with the most ductile fracture morphology, presenting equiaxed, homogeneously distributed dimples across the fracture surface (Figure 5.44 e). This is consistent with the highest transformation kinetics and full martensitic conversion, which, combined with multidirectional thermal dissipation, ensures minimal residual stress anisotropy and promotes uniform dislocation structures. In contrast, despite elevated transformation kinetics, the circular strategy displays the most brittle fracture features, including intergranular cracks and cleavage facets. This behavior stems from excessive heat accumulation and complex triaxial contraction near the periphery, which fosters carbide coarsening and δ -ferrite formation along grain boundaries. These microstructural instabilities, combined with high residual stresses, inhibit effective plastic deformation, resulting in premature failure.

5.5.5 Designing and modelling of advanced scanning patterns

After systematic learning from multiple deposition paths, two scanning strategies, S-pattern and a layer-wise mixed-pattern are designed to further understand the controlling elements of temperature distribution, phase transformation kinetics, and residual stress evolution. Figure 5.45 dictates the scanning path for these two proposed patterns. This study is performed through building a comprehensive experimental-numerical-machine learning framework that essentially defines the dilatometric curve for the proposed pattern. Layer-wise mixed-pattern alternates scan directions across successive layers (longitudinal, transverse and inclined), strategically balancing directional heat flow and mitigating the accumulation of

transformation-induced strain. Meanwhile, the S-pattern employs a continuous serpentine trajectory to ensure smoother heat input, minimizing thermal discontinuities between adjacent tracks.

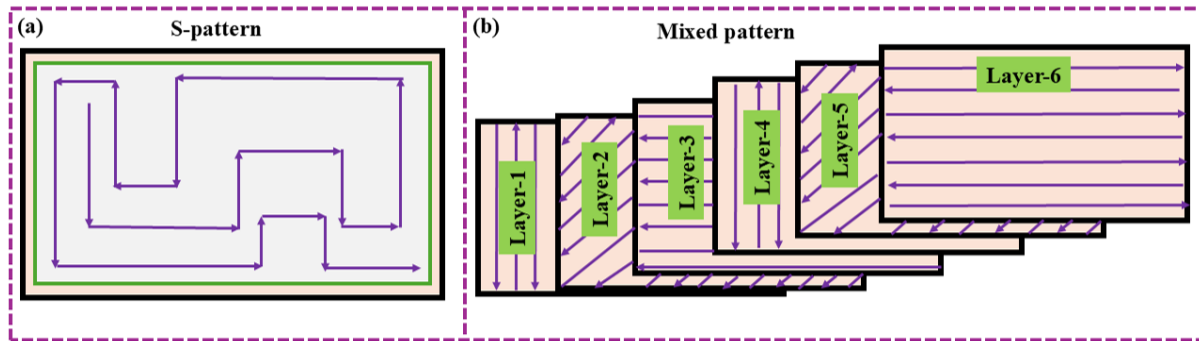


Figure 5.45: Illustration of the advanced scanning pattern utilized for printing rectangular components: (a) S-pattern and (b) Mixed pattern.

The strain-temperature curve of S-pattern and mixed-pattern are constructed from TCN model trained by experimentally measured dilatometric data. The thermal histories from high-fidelity simulations served as input features (temperature) for the TCN, allowing prediction of transformation strains under realistic deposition conditions. The arithmetic average values of transformation temperature from six dilatometric patterns are predefined for proposed patterns. Accordingly, the temperature history of the heating and cooling cycles for first layer deposition of proposed scan patterns is evaluated. The time-temperature data is captured for a fixed position of the deposited bead within the range of the average transformation temperatures. It is noteworthy that average heating and cooling rates over transformation temperature is fixed. Hence, the temperature profiles for the reconstruction of dilatometric curve also vary according to the deposited bead pattern. The dilatometric strains are then incorporated into a phase-aware mechanical framework to compute the evolution of residual stress, accounting for transformation plasticity and volumetric expansion. This approach highlights the potential of integrating data-driven models with physics-based simulations to design thermally balanced scan paths, ultimately improving the printability and structural integrity of DED components.

The effectiveness of TCN in predicting the dilatometric response is comprehensively demonstrated through both training diagnostics and experimental validation. Evolution of

RMSE over training epochs reveals a rapid decline during the initial learning phase, signifying efficient optimization and successful capture of temporal dependencies in thermal and process data. As training progresses, the RMSE stabilizes with minimal fluctuations, indicating reliable generalization. By the 30th epoch, the model achieves a training RMSE of approximately 0.0027 and a validation RMSE of around 0.0024, reflecting a well-regularized model with no signs of overfitting (Figure 5.46). This behavior highlights the strength of dilated causal convolutions in learning both local and long-range temporal patterns relevant to phase transformation phenomena. Further substantiating this performance, parity plots exhibit high predictive accuracy, with the training and testing datasets yielding R^2 values of 0.9742 and 0.9746, and corresponding RMSE values of 0.0031 and 0.0037, respectively (Figure 5.47). This strong generalization capability is further validated through a direct comparison of predicted and experimentally measured dilatometric strain for the inclined scanning strategy (Figure 5.48 a).

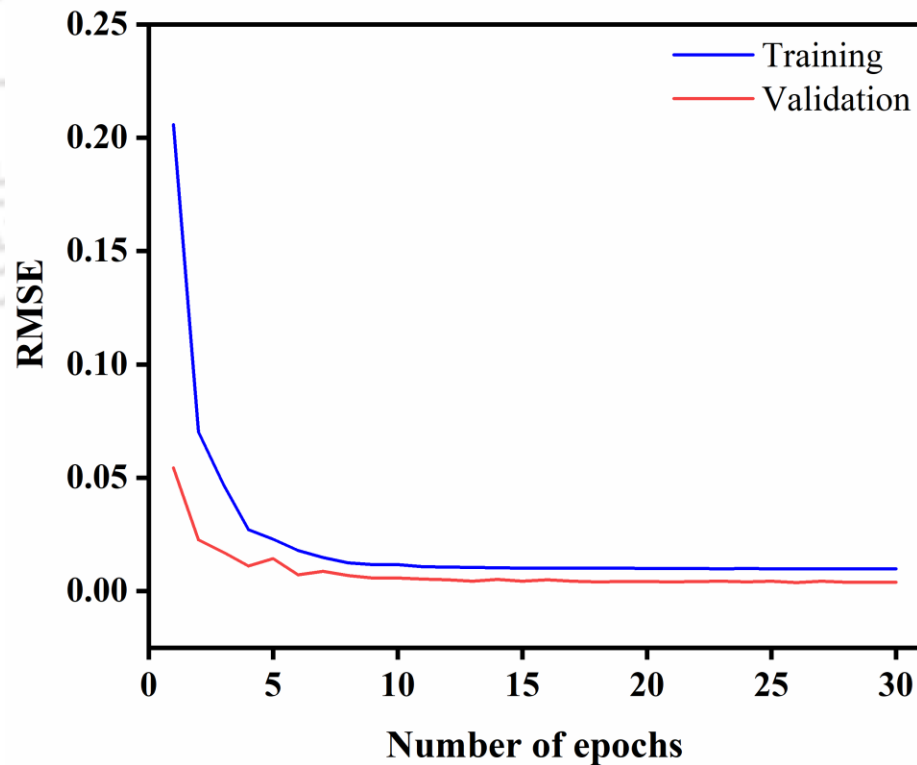


Figure 5.46: Training and validation RMSE loss curves for the Temporal Convolutional Network (TCN) model used to predict dilatometric strain, demonstrating model convergence and generalization performance.

In the complete thermal cycle, the TCN model closely tracks the strain evolution, with accurate representation of both thermal expansion during heating and contraction during cooling. Notably, at approximately 780°C, the experimental strain peaks at 0.0027, while the model predicts 0.0026, yielding a marginal error of about 3.7%. The model also effectively captures the nonlinear increase in strain associated with martensitic transformation within the 800–900 °C range, where it predicts a peak strain of 0.0033 against the experimental maximum of 0.0034. During cooling, both predicted and experimental curves exhibit sharp reductions in strain due to thermal contraction and reverse transformation, concluding with highly consistent final values.

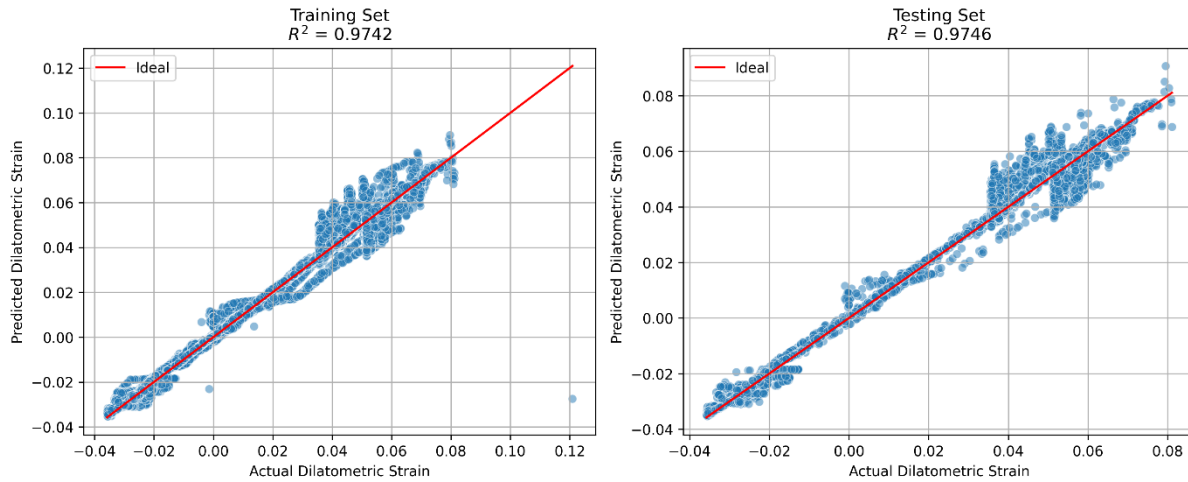


Figure 5.47: Comparison between TCN model predicted and experimental measurements of dilatometric strain for both training and testing datasets, showcasing the model’s high predictive accuracy and robust generalization across unseen thermal profiles.

The predicted dilatometric strain evolution for the S-pattern and mixed-pattern scanning strategies by TCN model are depicted in Figure 5.48 b. For the S-pattern, the dilatometric strain increases steadily during the heating cycle and attains a peak value of approximately 0.070 near 1100 °C. This behavior reflects uniform thermal exposure and relatively moderate thermal gradients. As cooling progresses, the strain exhibits a smooth and gradual decrease, reaching around −0.035 at the end of the thermal cycle. This moderate contraction suggests a relatively controlled martensitic transformation, typical of scanning strategies with balanced heat distribution and moderate cooling rates. In contrast, the mixed pattern reveals a marginally

higher thermal expansion during the heating phase, with a maximum strain of nearly 0.075 observed around 1120 °C. The difference in thermal response arises from intensified energy deposition and more complex melt pool interactions inherent to this strategy. Upon cooling, the mixed-pattern undergoes a steeper drop in dilatometric strain, reaching a minimum of approximately -0.052 . This rapid contraction reflects a more aggressive martensitic transformation, influenced by higher thermal gradients and faster cooling conditions. Notably, in the temperature range of 450°C to 700°C, which is critical for transformation kinetics, the mixed-pattern exhibits a sharper inflection, signifying a more abrupt onset of phase change compared to the S-pattern.

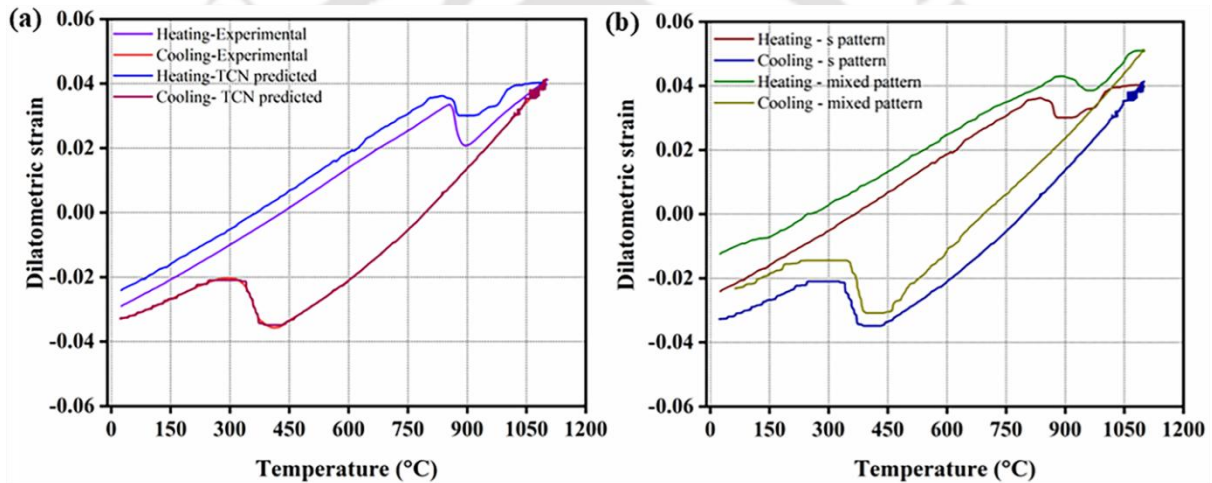


Figure 5.48: (a) Comparison of TCN-predicted and experimentally measured dilatometric strain for the inclined pattern; (b) TCN-predicted dilatometric strain profiles for S and mixed patterns.

3D simulated reveals distinct thermal fields for the S pattern and mixed pattern scanning strategies during final layer deposition Figure 5.49 (a and b). In the S pattern, a larger molten pool and a visibly broader mushy zone, bounded by the liquidus (1500°C) and solidus (1420°C) temperatures, indicate a more gradual thermal gradient and extended solidification interval. Notably, the S pattern produces a larger molten pool, and a visibly thicker mushy region compared to the mixed pattern. This expanded mushy zone in the S pattern indicates a broader transition region between liquid and solid phases, reflecting a more gradual thermal gradient that may have critical implications for solidification dynamics and phase

transformation pathways. After the completion of the final layer and a subsequent cooling phase lasting approximately 1100 s, the temperature across the entire component returns to ambient conditions (25 °C), ensuring thermal equilibrium. Transient thermal profiles further illustrate the divergence in thermal behavior. The S pattern demonstrates a stable thermal response, reaching a peak temperature of approximately (Figure 5.49 c) reaching a peak temperature of approximately 955 °C and cooling smoothly to around 455 °C, consistent with uniform heat dissipation. Conversely, the Mixed pattern shows thermal instability, with a rapid peak near 1047 °C followed by a steep decline to approximately 324 °C and a prolonged cooling to about 37 °C. These thermal disparities are mirrored in the phase transformation kinetics (Figure 5.49 d). In the S pattern, rapid martensitic transformation initiates immediately after solidification, with the martensitic fraction rising from 0.00 to approximately 0.89 within 25 s, while the austenitic fraction drops from 0.92 to 0.03. This behavior, driven by a steep and consistent cooling trajectory, results in homogeneous martensitic evolution with minimal retained austenite. In contrast, the Mixed pattern exhibits a delayed transformation, beginning only after 40 to 50 s and reaching a final martensitic fraction of approximately 0.85 by 160 s. The gradual decrease in austenite, from 0.92 to 0.07, reflects spatially varied cooling and incomplete transformation. This nonuniform transformation increases the likelihood of austenite retention, phase mismatch, and elevated residual stress. Overall, the thermal and phase transformation analyses underscore the critical influence of scan strategy on solidification dynamics, transformation strain accommodation, and the resulting structural integrity of additively manufactured components.

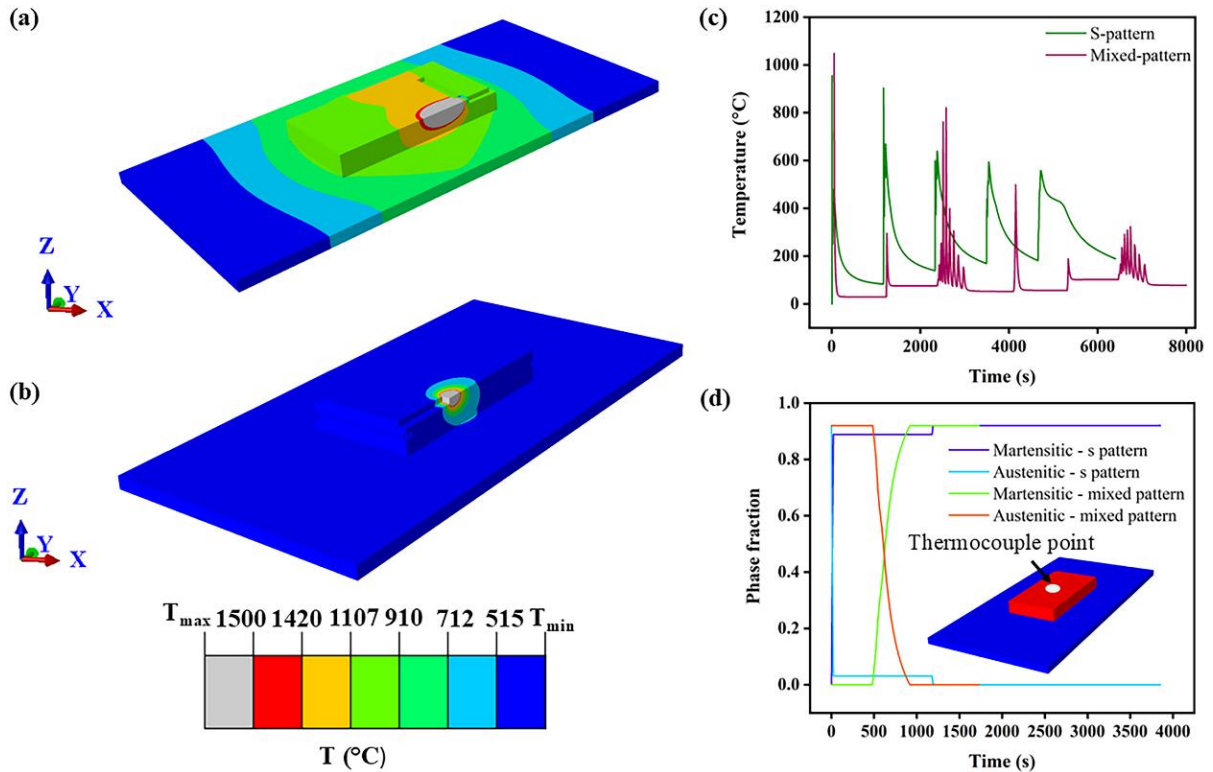


Figure 5.49: (a, b) Simulated 3D temperature profile of S and mixed pattern; (c) transient thermal profiles; and (d) Evolution of austenitic and martensitic fractions for both patterns.

Computed Von Mises stress distributions for the S-pattern and Mixed-pattern scanning strategies reveal distinct residual stress localization, closely linked to their thermal and transformation histories. For the S-pattern, the maximum equivalent stress ($S_{max} = 586.8 \text{ MPa}$), while the minimum stress ($S_{min} = 13 \text{ MPa}$). High tensile residual stresses are predominantly concentrated near the clamping points, where mechanical constraints hinder free contraction during cooling (Figure 5.50 a). This stress localization correlates with the higher K_m (1.1), calculated for S-pattern, which reflects a rapid and uniform martensitic transformation, as previously shown in the phase evolution profile. The swift transformation induces significant volume expansion due to shear-driven phase change, yet the consistent thermal gradient allows partial accommodation of transformation strains, limiting the spread of residual stress within the deposited region. In contrast, mixed pattern exhibits a slightly higher maximum Von Mises stress of 617.6 MPa, with a minimum stress value of 6 MPa (Figure 5.50 b). The tensile residual stresses are prominently observed near the substrate–deposition interface, indicating strong stress buildup in the heat-affected zone. This intensified

stress field can be attributed to the lower K_m (0.7), signifying a slower, more heterogeneous martensitic transformation. The two-stage cooling behaviour, combined with uneven phase evolution, limits the capacity for transformation-induced strain relief. Consequently, the retained austenite and differential thermal contraction across regions exacerbate stress accumulation, particularly in constrained zones of the substrate. These findings confirm that higher K_m values indicative of effective transformation-induced plasticity, and promote more uniform stress redistribution, whereas lower K_m leads to stress concentration due to incomplete or delayed transformation.

The residual stress distributions along the longitudinal and transverse directions, shown in Figure 5.50 (c and d), demonstrate a strong correlation with the kinetics of martensitic transformation and the associated TRIP. In the S-pattern, both stress components exhibit oscillatory behavior, with peak longitudinal residual stress reaching ~ 244 MPa and transverse stress peaking at ~ 96 MPa. These elevated stresses arise from the abrupt martensitic transformation that occurs within a narrow thermal window, as indicated by high K_m (Figure 5.50 c and e). This parameter reflects a steep transformation strain rate per unit temperature, driven by rapid cooling. The resulting phase transformation strain, associated with the shear-dominant lattice change from austenite to martensite, induces localized expansion. In contrast, the mixed pattern shows a markedly different stress profile, with the longitudinal stress peaking at a lower value of ~ 215 MPa, and the transverse stress significantly reduced to ~ 11 MPa (Figure 5.50 d and e). These differences are directly attributable to the slower and more spatially heterogeneous martensitic transformation, as quantified by a lower K_m .

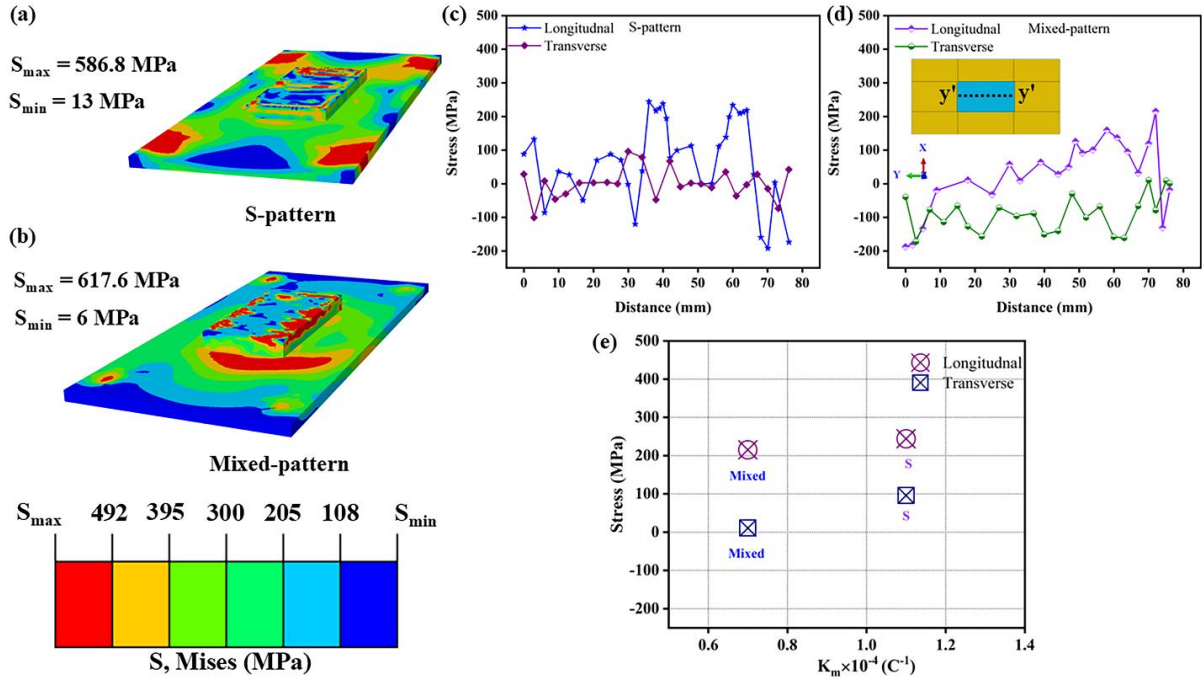


Figure 5.50: (a, b) Simulated 3D Von Mises stress distribution for S and mixed pattern; (c, d) variation of longitudinal and transverse residual stresses along the longitudinal direction of printed rectangular plate; (e) Correlation of maximum longitudinal and transverse residual stresses with K_m for both patterns.

5.5.6 Summary

The current investigation focuses on the development of a comprehensive framework to tailor residual stress in wire-based DED of ferritic steel by integrating systematic experiments with AI-driven thermo-mechanical modelling. Residual stress generation is one of the most persistent challenges in additive manufacturing of ferritic–martensitic steels such as 9Cr–1Mo, which are widely used in high-temperature AUSC power plant applications due to their excellent creep resistance, oxidation resistance, and structural stability. However, during DED, repeated thermal cycling and steep thermal gradients lead to non-uniform solid-state phase transformations, most notably the austenite to martensite transformation that couples directly with residual stress evolution. The accumulation of high tensile residual stresses not only compromises dimensional accuracy and fatigue life but also promotes Type IV cracking along fine-grained heat-affected zones, thereby limiting the reliability of ferritic steel components in service. Addressing these issues demands a multi-scale approach that couples experimental

insights with predictive models capable of capturing the intricate interplay between thermal history, phase transformation kinetics, and mechanical stress generation.

On the experimental front, wire-based DED of 9Cr–1Mo steel are conducted in multiple configurations including single-track, single-layer, multi-layer thin walls, and multi-track multi-layer builds. Six distinct scanning strategies longitudinal, transverse, inclined, spiral-in, spiral-out, and circular are employed to systematically modulate thermal gradients and evaluate their impact on microstructure and stress fields. Dilatometric experiments are carried out to quantify transformation-induced strain during controlled heating and cooling cycles, providing critical input for TMM models. Complementary characterization techniques including XRD, residual stress analysis, EBSD and TEM are used to map martensitic transformation, lath morphology, dislocation substructures, and carbide precipitation. Mechanical testing through tensile and microhardness measurements confirms the structural integrity of the deposits and establishes direct links between scan strategy, residual stress magnitude, and macroscopic performance.

Parallel to experiments, FE based TMM simulations are developed to capture the coupled phenomena governing stress generation. A double-ellipsoidal heat source model calibrated against single-bead trials is employed to simulate heat input. While element birth–death techniques mimic sequential material deposition. The FE framework incorporates temperature-dependent properties of ferritic steel, phase transformation strains derived from dilatometry, and boundary conditions representative of real DED experiments. This enables prediction of transient temperature distributions, martensitic phase fractions, and stress evolution across the deposited geometry. While such high-fidelity simulations are indispensable for mechanistic understanding, they are computationally expensive, especially when exploring wide process design spaces involving multiple scan strategies and dwell time variations.

The combined experimental–numerical–AI framework is applied to the design of advanced scan patterns. Analysis of the six conventional strategies reveals that the inclined path offers superior mechanical response with ultimate tensile strength of 1587 MPa and elongation of 19.1% while maintaining moderate residual stress (~411 MPa), whereas the circular scan path induces the highest tensile stress (~628 MPa) despite acceptable bead geometry. These results underscore the trade-offs between microstructural refinement, mechanical performance, and residual stress that must be balanced in scan path design.

Learning from these findings, two advanced hybrid strategies are proposed: an S-pattern and a layer-wise mixed pattern that combine directional modulation with localized heat redistribution. By integrating TCN-predicted transformation strains into the FE-TMM model, these strategies are computationally evaluated before experimental validation. The mixed pattern is identified as the most effective, achieving residual stress reduction to ~ 278 MPa while promoting smoother and more uniform martensitic evolution across layers. XRD measurements confirm the numerical predictions, while EBSD phase maps reveal a refined lath martensite structure with reduced dislocation tangles and more homogeneous carbide precipitation.





Conclusions and Scope of Future Work

6.1 General background

Residual stress management is a critical challenge in wire-based DED of ferritic steels, particularly 9Cr–1Mo, which are widely employed in high-temperature energy applications owing to their creep resistance and structural stability. The steep thermal gradients, cyclic reheating, and rapid solidification inherent to the DED process often result in heterogeneous microstructures and significant tensile residual stresses. These stresses not only degrade dimensional accuracy and mechanical performance but also accelerate failure mechanisms such as Type IV cracking, thereby limiting the reliability of additively manufactured components. Over the years, several empirical and analytical models have been proposed to explain residual stress development in laser and arc-based additive processes. However, these approaches have shown limited accuracy and general applicability due to the complexity of coupled thermo-metallurgical-mechanical interactions. To overcome these limitations, recent advances have turned toward integrating high-fidelity FE models, experimental validation, and AI frameworks. Such hybrid approaches offer the dual advantage of mechanistic understanding and computational efficiency, allowing both forward predictions of stress evolution and inverse design of deposition attributes.

6.2 Conclusions

Through the integration of a comprehensive literature review, systematic experimental studies, and AI-enabled thermo-mechanical modelling, this work tackles the fundamental challenge of residual stress evolution in wire-based DED of 9Cr-1Mo steel. Special emphasis

is placed on establishing a holistic framework that couples experimental insights, high-fidelity FE simulations, and AI surrogates to decode the complex interrelationships among thermal history, dwell time, scanning strategy, and residual stress development. By integrating predictive algorithms with experimentally validated process data, the work transcends conventional empirical approaches and demonstrates how intelligent process design supported by advanced AI tools can actively tailor residual stress distribution. In particular, the focus is on optimizing deposition attributes and advanced scanning strategies to mitigate tensile stress, refine microstructures and enhance mechanical reliability of 9Cr–1Mo steel components intended for high-temperature structural applications. The key findings from this study are as follows:

- The literature review illustrates that residual stress evolution in ferritic/martensitic steels such as 9Cr-1Mo is primarily governed by deposition attributes, thermal profiles, and phase transformation kinetics during wire-based DED process. Available empirical and analytical models are limited in predictive accuracy, underscoring the need for integrated frameworks combining experiments, numerical simulations, and AI-driven approaches.
- A thermo-mechanical model is developed in this respect and tested with experimental data of temperature profile and residual stress. The FE based simulations successfully captured spatiotemporal temperature evolution and residual stress distribution in wire-based DED process. The reliable temperature histories from thermal simulation is successfully used for microstructural and residual stress analysis.
- The thin wall structure and multi track-multi layers deposition defined by various scanning patterns are fabricated in the current study following wire based DED of 9Cr-1Mo steel. The temperature using thermocouple and residual stress are experimentally measured. The characterization of microstructure and mechanical properties of the deposits are evaluated.
- Results highlighted that tensile residual stresses increase sharply with prolonged dwell times, while optimized inter-layer dwell time strategies and scanning strategies modulation reduce stress magnitudes and improve structural stability. The longitudinal stress along the build direction is highly sensitive to inter-layer dwell time, making it a key design factor. A shorter dwell time of 50 s reduces the maximum inter-pass temperature from 413.4°C to 25.9°C, which helps to lower tensile residual stress. On the other side, increasing the dwell time from 50 s to 500 s raises residual stress significantly, from 95.3 MPa to 634.8 MPa.

- In bi-directional scanning, higher cooling rates ($\sim 2814^{\circ}\text{C/s}$) initially dissipate heat faster, but heat accumulates over time, elevating inter-pass temperatures. This inhibits full martensitic transformation, leading to a lower martensitic fraction (97.5%). A reduced martensitic fraction decreases volumetric strain from phase transformation, which lowers tensile residual stress (~ 492 MPa) due to less internal expansion. Research indicates that linear energy density is key in managing the development of tensile residual stress and minimizing distortions along the deposition height in the final printed components when using the bi-directional deposition method.
- The incorporation of phase transformation kinetics significantly improved stress predictions, revealing the critical role of martensitic transformation-induced strain in stress accumulation and relaxation. TMM model which includes the effect of phase transformation kinetics accurately predicted residual stress magnitude for each of the scanning strategies. Particularly, the longitudinal residual stresses predicted for each of the scanning strategies are 628 MPa for circular scanning, 527 MPa for longitudinal scanning, 239 MPa for spiral-in scanning, and 278 MPa for scanning using a mix of circular and longitudinal scanning.
- Physics-informed deep learning (PIDL) models trained on FE and experimental datasets achieved high accuracy in forward prediction of transient thermal fields. Recurrent DL models (LSTM, Bi-LSTM, GRU, TCN) effectively captured the sequential evolution of residual stresses, with TCN showing the highest fidelity. The AI models are also used for backward prediction of deposition attributes such as power, velocity, and inter layer dwell time from targeted thermal or stress threshold.
- The PIDL model shows reasonable accuracy in predicting non-linear temperature and residual stress profiles for both interpolated and extrapolated dwell times. For dwell time 180 s to 270 s, the temperature drops from 86°C to 47°C and the slight increase in stress from 618 MPa to 630 MPa are observed. In extrapolated cases (450 s and 500 s), the PIDL model accurately predicts inter-pass temperature stabilizing at 30°C (near ambient temperature), with minor deviations in residual stress at 500 s, ensuring reliable performance even beyond the training range.
- A TCN model trained on experimental dilatometry successfully predicted phase transformation strain evolution enabling residual stress estimation via coupled FE

simulation. This generated dilatometry curve is further used to design advanced scan patterns and their prediction of residual stress evolution using FE based TMM model.

- The deposition following uni-directional strategy possesses more ductility than bi-directional scan, however, less than wrought steel. Bi-directional scan shows superior tensile strength than uni-directional scan, however, both strategies result in significantly higher strength than base material. The formation of carbides ($M_{23}C_6$ and MX) and its uniform distribution mainly serve the strengthening mechanism.
- The thin-wall fabricated by using the CMT-based DED process exhibits a heterogeneous microstructure consisting of a lath martensitic matrix, δ -ferrite, and carbide precipitates ($M_{23}C_6$ and MX).
- The fracture analysis reveals mixed mode failure characterized by dimples, cleavage facets, and tear ridges, influenced by residual stress and microstructural heterogeneity. The fracture transits from quasi-cleavage to ductile failure as the scanning strategy changes from uni-directional to bi-directional.
- EBSD analysis confirmed >99% martensitic content (BCC/BCT), with inclined and spiral-in strategies reducing grain orientation spread (GOS) and dislocation density. XRD patterns validated dominant BCC phase via $\{110\}$, $\{200\}$, and $\{211\}$ reflections, supporting full transformation.
- Overall, this study establishes a holistic methodology that integrates experimental insights, high-fidelity simulations, and AI surrogates to enable intelligent process design for residual stress management in 9Cr-1Mo steel.

For AUSC power systems employing 9Cr–1Mo steel where residual stress-induced Type IV cracking poses significant reliability concerns the scanning strategy-driven approach demonstrated in this study offers a robust pathway to enhance the printability, structural integrity, and service life of DED-fabricated components. Beyond 9Cr–1Mo steel, the proposed framework is equally applicable to other advanced engineering materials such as H13 tool steel, 17-4 PH stainless steel, Ti-6Al-4V alloy, and nickel-based superalloys commonly used in aerospace and high-temperature applications, where controlling thermal gradients and transformation-induced stresses is critical for ensuring performance and durability.

6.3 Application Potential and Scope of Future Work

Some of the essential attributes are worthwhile to investigate further and are expected to be the future scope of work for the expansion of its application potential:

- The developed hybrid framework, though demonstrated for wire-based DED of ferritic steel, can be extended to other AM variants such as laser-based DED, laser powder bed fusion (LPBF), and selective laser melting (SLM). A comparative study across these processes will reveal how differences in energy source, powder or wire feed, and thermal history affect residual stress distribution and structural integrity.
- The present study established a strong correlation between deposition attributes and stress evolution. However, the effect of alloy-specific features and microstructural refinement has not been fully integrated into the predictive models. Exploring these metallurgical effects experimentally and numerically will help extend the framework to broader alloy families including stainless steels, nickel superalloys, and titanium alloys.
- While TCN have shown high accuracy for residual stress prediction, the deployment of more advanced AI techniques such as generative models (GANs, diffusion models) can be explored. These models can create synthetic thermal–stress histories and propose novel scan strategies beyond conventional human design, significantly accelerating process innovation.
- The current framework has primarily relied on offline datasets generated from experiments and FE models. Coupling AI models with in-situ monitoring tools (thermal imaging, acoustic emission, and digital image correlation) can enable real-time adaptive control of stress evolution, paving the way for closed-loop manufacturing systems.
- Finally, the robustness of the developed models can be validated through the creation of digital twins of AM processes. Such digital replicas, embedding both FE-based physics and AI surrogates, can serve as predictive tools for industrial-scale applications, reducing qualification time and cost while improving confidence in the deployment of additively manufactured ferritic steel components.

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List of publications out of present work

International Journals

1. **Amrithesh Kumar**, Ritam Sharma, Swarup Bag, Vikas Chandra Srivastava, Sajjan Kapil (2023), “Physics-informed machine learning models for the prediction of transient temperature distribution of ferritic steel in directed energy deposition by cold metal transfer” **Science and Technology of Welding and Joining** (Taylor and Francis), 28, 914-922.
- *2. **Amrithesh Kumar**, Debtanay Das, Nikhil D Raj Swarup Bag, Vikas Chandra Srivastava (2025), “Comparison of machine Learning performance for the prediction of melting efficiency and bead Geometry in wire arc additive manufacturing process” **Archives of Metallurgy and Materials** (Applied sciences), 70, 1, 29-38 .
3. **Amrithesh Kumar**, Swarup Bag, Vikas Chandra Srivastava (2024), “Role of inter-layer dwell time on residual stress generation of a thin wall structure by directed energy deposition of ferritic steel” **Materials Chemistry and Physics**, (Elsevier), 340 130807.
4. **Amrithesh Kumar**, Swarup Bag, Vikas Chandra Srivastava (2025), “Bi-directional scanning strategies for residual stress management by tailoring microstructural evolution in directed energy deposition of 9Cr-1Mo steel” **Journal of Materials Processing Technology**, (Elsevier), 341, 118906.
5. **Amrithesh Kumar**, Swarup Bag, Vikas Chandra Srivastava (2025), “Development of temporal convolutional neural network model for the prediction of residual stress in directed energy deposition process” (Under review).
6. **Amrithesh Kumar**, Swarup Bag, Vikas Chandra Srivastava (2025), “Tailoring martensitic transformation and residual Stress in arc-DED fabricated 9Cr-1Mo Steel: A scanning strategy-driven multi-scale experimental and computational study” (Under review).
7. **Amrithesh Kumar**, Antara Parui, Hrishi Inani, Swarup Bag, Vikas Chandra Srivastava (2025), “Correlation-guided temporal deep learning model for the prediction of fatigue life of printed AlSi10Mg alloy” (Under review).

8. **Amritesh Kumar**, Swarup Bag, Vikas Chandra Srivastava (2025), “Elucidation of mechanical characteristics of 9Cr-1Mo steel through deep learning models for different scan patterns” (Under preparation).

9. Pankaj Kumar, **Amritesh Kumar**, Santosha Kumar Dwivedy, Subham Banerjee (2025), “Integrated machine learning approach for final weight prediction in stimuli-response 4D printed single-layer elastomer strip”, **Engineering Application of Artificial Intelligence** (Elsevier), 162, 112756.

10. Pankaj Kumar, **Amritesh Kumar**, Santosha Kumar Dwivedy, Subham Banerjee (2025) Machine Learning guided tuning of shape memory behavior printed single layer elastomer strip for smart drug delivery”, 4D printing Journal.

International Conferences

11. **Amritesh Kumar**, Swarup Bag, Vikas Chandra Srivastava, M.Ruhul Amin (2022) “Thermo-mechanical behaviour of multi-layer deposition for wire arc additive manufacturing of structural steel: wire arc additive manufacturing” (**IMECE2022-88917, ASME 2022 International Mechanical Engineering Congress & Exposition**).

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