

Finite element simulation of the Direct Energy Deposition using Comsol Multiphysics

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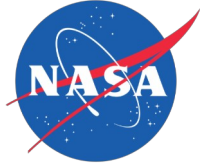
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Summary

Direct Energy Deposition (DED) is an emerging technology extensively employed in metal Additive Manufacturing (AM). Despite its widespread industrial application, mathematical modeling in this domain remains challenging. This complexity arises from the intricate nature of the modeling approach and the nonlinear behavior of material parameters across a broad temperature range. Consequently, experimentalists often resort to a trial-and-error method to achieve structures with desired properties. However, this approach can be time-consuming and may not always yield parts with the requisite characteristics, highlighting the necessity for mathematical modeling to enhance manufacturing success.

This study focuses on thin-walled manufacturing with a single bead thickness, adjusting laser parameters to produce such structures. The laser cladding speed, typical for DED manufacturing, is considered to be on the order of centimeters per second. The various wall thicknesses and heights are explored to discern the general characteristics of walls manufactured via this DED approach.

Our modeling approach diverges from the conventional DED modeling based on activation-deactivation of predefined mesh domains, commonly implemented in many finite element codes. Instead, a method is proposed that effectively models layer cladding and melt pool dynamics, enabling predictions of the microstructure in the resulting structures. The formation mechanisms of cellular, dendritic columnar, and stray (equiaxed) grains, which arise from the interplay between nucleation and growth from the surface is analyzed.

The study also examines the feasibility of microstructure formation to demonstrate the various thermal characteristics inherent in wall manufacturing. Our results illustrate how different process parameters influence the temperature gradient and cooling rate of the molten pool, subsequently affecting the primary dendrite arm spacing (PDAS). This modeling technique allows for the investigation of diverse thermal conditions, facilitating the prediction of microstructure and residual stresses in the manufactured parts.

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1 Introduction

Direct Energy Deposition (DED) is a newly developed technology extensively utilized in metal additive manufacturing (Ref. 1–8). This technology involves depositing powder onto a workpiece and melting it using an energy source. While various energy sources like lasers and electron beams can be used for material addition, the formation of layers remains a critical area of study, reflecting its significance in manufacturing processes. Despite its widespread industrial application, mathematical modeling in DED is still limited due to the complexity of the approach, which involves multiple physics phenomena and nonlinear material parameters across a broad temperature range.

DED is a metal deposition technique where a laser-melted powder stream is used to create a three-dimensional structure. This process, from the laser’s interaction with the powder to material solidification, requires meticulous consideration due to its complex physics. Numerous approaches have been developed to model this phenomenon. In our approach, we account for material addition, structure shape formation, and nonlinear material parameters over a wide temperature range, covering both solid and molten states.

COMSOL Multiphysics stands out as a robust simulation software designed for multi-physics modeling using the finite element method. Its strength lies in its ability to integrate multiple physics seamlessly, allowing for intricate modeling of complex phenomena (Ref. 9). In this report, the COMSOL software is employed to model DED additive manufacturing of INCONEL 625 material, focusing on thin wall formation. The DED process under consideration uses a laser heat source to melt a powder stream supplied to the solid surface, creating a melt source on the wall’s top and leading to free boundary motion due to the cladding procedure.

Thin-walled structures, crucial in industries such as aerospace, present unique challenges in additive manufacturing due to the complexities associated with AM constraints and limitations. Microstructure emergence and residual stress distributions are central to DED AM processes (Ref. 8, 10–12). Moreover, understanding the impact of varying process parameters – such as scan speed, laser power, and feed rate – is pivotal in determining the final part’s properties, necessitating a comprehensive mathematical model of DED processes.

Recently, the concept of Digital Twins (DT) has emerged as a method to create models that mirror the manufacturing workflow, aiding in the understanding, analysis, and improvement of fabricated items (Ref. 13). DT models show great promise in enhancing AM technologies, including process simulation, and can help to deeply understand the physics phenomena of manufacturing processes. The finite element analysis (FEA) developed within COMSOL can be seen as a simplified DT of the DED process, though it may not universally apply to all DED simulations.

Various DED modeling strategies have been explored in the literature, with successful applications in diverse cases. Notable commercial codes like Ansys Additive (Ref. 14), 3dExperience (Ref. 15), and Simufact (Ref. 16) have been widely recognized in research and industry. Our innovation within COMSOL involves developing unique approaches that diverge from standard activation-deactivation techniques (Ref. 12, 14–17).

This report outlines frameworks for investigating DED processes, encompassing process simulation models based on heat transfer for both melt and solid phases, as well as the evolution of the free boundary of the cladding melt during DED, and studies on residual stresses. The simulation model presented is simple, facilitating predictions of time history, cooling rates, thermal gradients, microstructure, and morphology during DED manufacturing. These models utilize material data and process parameters to accurately reflect Additive Manufacturing technology, with numerical

simulation outcomes bolstered by fundamental physics processes and corresponding experimental validations. However, it is important to note that our analysis does not incorporate the influence of the build plate, which may significantly impact DED manufacturing. Our primary focus remains on the wall structures themselves, with particular attention given to the corresponding boundary conditions at the base of the walls.

2 Governing Equations

This report focuses on developing models that elucidate various phenomena observed in DED processes, rather than simulating specific experiments. Our approach aims to deepen understanding of the physics underlying the material cladding process, providing insights into the simulation results. The versatility of the analysis tools available in Comsol Multiphysics allows for an extensive exploration of the DED process, shedding new light on this technologically progressive method.

2.1 Liquid-Based DED Simulation Approach

The DED process is fundamentally thermal in nature, thus making the heat transfer equation a cornerstone of its physical simulation. In this regard, the thermal conductivity equation (1) is utilized to articulate the energy balance within the selected physics domain. The equation's right-hand side accounts for the change in temperature per unit time within a volume, while the left-hand side encompasses both diffusive and convective heat flows. This includes all potential heat sources (Q) involved in the process.

As the material undergoes phases of solidification and cooling, thermomechanical modeling becomes critical to account for the stresses and strains that develop during the formation of structures. Nevertheless, simplicity in modeling is often preferred for more straightforward results interpretation. Therefore, the general strategy is to integrate the essential physics needed to effectively model the DED process, as recommended in literature (Ref. 1, 9). The energy balance for heat transfer, as considered in our model, is encapsulated by the equation governing the domain temperature (T). This approach provides a comprehensive understanding of the thermal dynamics within the DED process, crucial for optimizing manufacturing outcomes and predicting the properties of the fabricated parts

$$\rho(T)C(T)u\nabla T + \nabla(\lambda(T)\nabla T) + Q = \rho(T)C(T)\frac{\partial T}{\partial t} \quad (1)$$

Here $\rho(T)$, $C(T)$ are density, specific heat capacity, u fluid velocity, ∇ is the divergence operator, and Q is the heat source. All specific material parameters are determined in all temperature range for a solid and melt state. The boundary condition involves convective heat transfer and radiative heat transfer

$$q + q_r + q_c = \frac{\partial T}{\partial n}. \quad (2)$$

The thermal energy source utilized during Directed Energy Deposition in this report is represented using a heat flux model. Heat flux models find widespread application in various thermal processes (Ref. 9). In the the Gaussian function used here the size of the melt pool is denoted by the radius r_0 . In a laser based DED process as the input heat q may be considered as the Gaussian heat distribution:

$$q(x, y) = 2q_0/(\pi r_0^2)\exp(-2(x^2 + y^2)/r_0^2), \quad (3)$$

where $q(x, y)$ is the absorbed surface power, and x, y are Cartesian coordinates on the surface, q_0 is the laser average power. The radius r_0 is taken at which the intensity drops to $1/e^2$ (about 13.5%) of its peak value.

For q_r , q_c the next equations are given

$$q_r = \sigma \epsilon (T^4 - T_0^4), \quad (4)$$

$\epsilon = 0.5$ is the material emissivity, $\sigma = 5.67 \times 10^{-8} \text{ W/(m}^2 \text{K}^4)$ is the Boltzman constant, and $T_0 = 300 \text{ K}$ is the ambient temperature

$$q_c = h(T - T_0), \quad (5)$$

where h is the heat convection coefficient ($\text{W/m}^2 \text{K}$), the bottom surface for the all simulations is taken at the constant temperature T_0 , say room one.

In COMSOL, the Heat Transfer module distinctly addresses the heat transfer problems in solid and liquid phases. Specifically, for the liquid phase, heat transfer can be intricately linked with a phase transition function, facilitating a smooth solid-to-liquid transition. In this scenario, material properties undergo continuous changes within the transition range, with the latent heat being integrated into the heat capacity. The phase change is triggered by temperature variations in the transition zone, leading to abrupt changes in material properties. Notably, the solid-to-liquid transition culminates in a sharply defined transition between solidus and liquidus temperatures, which is very important for accurately determining the locations of free boundaries.

2.2 Solid-Based DED Simulation Approach

In the context of solid-state heat transfer problems, similar simulation results can be attained. For this approach, it's imperative to precisely define thermo-physical material parameters such as heat capacity and conductivity.

Contrasting with the liquid-based approach where the entire domain is treated as a liquid state frozen below the melting temperature, the solid-based approach regards the entire domain as solid. When the temperature surpasses the melting point in this approach, the solid assumes liquid properties. The transformation from solid to liquid phase is modeled by modifying the specific heat to include an additional latent heat term (See, for example, (Ref. 18)):

$$C(T) = C_p(T) + L_m \frac{1}{\sqrt{\pi \Delta T^2}} \exp \left(-\frac{(T - T_m)^2}{\Delta T^2} \right), \quad (6)$$

where $C_p(T)$ represents the specific heat in the solid state, L_m is the latent heat of the solid-liquid phase transition, ΔT is the interval of solidification, and T_m is the melting temperature. A graphical representation of the function $C(T)$ employed in this report is presented in the appendix.

The results of the simulation using the solid-based domain are compared with those from the liquid domain simulation (1) and are showcased in Figure 1. General similarities are observed in the 3D contour plots of both approaches. To corroborate these findings, the temperature distribution along the path on the middle of the top surface during the laser scanning process is depicted in Figure 1. This comparison confirms that the solid-based and liquid-based approaches yield similar outcomes, demonstrating their effectiveness in modeling the complexities of the DED process.

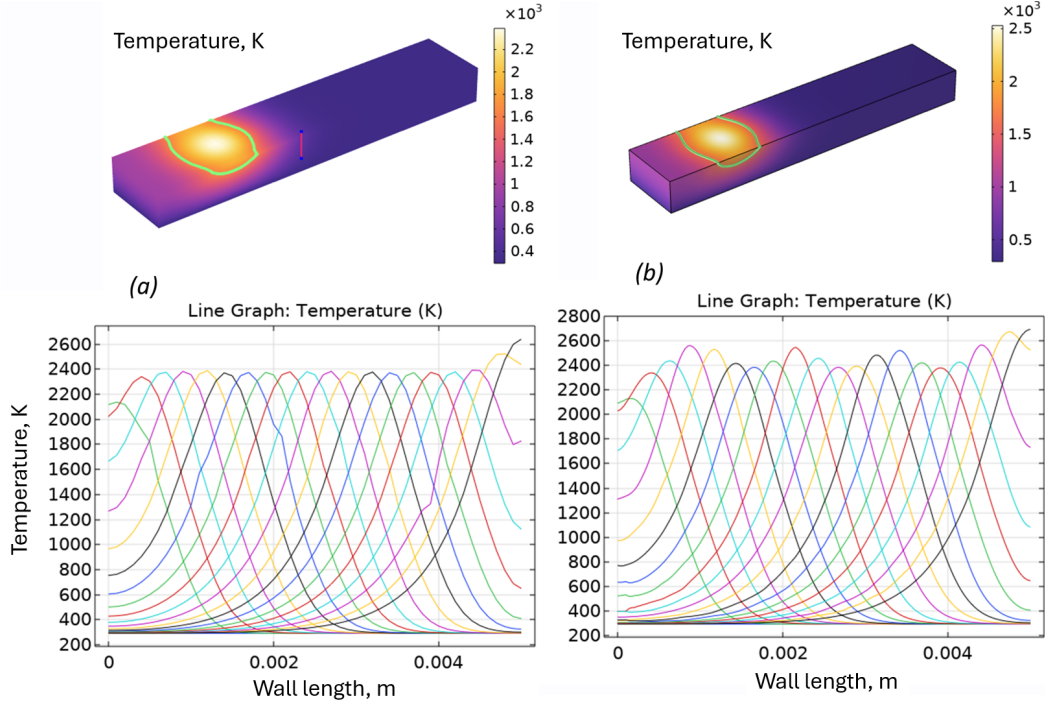


Figure 1.—Comparison the results for liquid based model – a) and solid one – b) for: $q_0 = 1.5e8 W/m^2$, $t=0.125$ s. The contour plot temperature distributions are presented in the first row and line plots of the temperature along the middle line located on the top surface along the laser scan path are presented in the second row.

2.3 Lagrangian-Eulerian (ALE) method

In the course of cladding, the subsequent process of added powder deserves consideration. COMSOL, through its implementation of the Arbitrary Lagrangian-Eulerian (ALE) method, offers an approach to account for material deformation. This is particularly valuable for modeling surface deformation during cladding and changes in the melt pool boundary. Utilizing free and mobile surfaces within an ALE deformable domain, the model effectively tracks the molten state of the material throughout the cladding process (Ref. 9).

The model takes into account the phase transition at the solid-melt interface, and the addition of mass mirrors the process of supplying the molten state to the free surface. To align the boundary evolution with experimental data, certain adjustable parameters for free boundary evolution are introduced.

It should be noted that physics' partial differential equations like equation (1) are typically framed in one of two ways: either within a fixed spatial coordinate system (Eulerian formulation), where the coordinate axes are stationary, or within a material coordinate system (Lagrangian formulation), attached to the material as it deforms, moving with it in its reference configuration. The pure Eulerian formulation faces a challenge when dealing with moving domain boundaries because it references physical quantities to fixed points in space, while the set of spatial points within the domain boundaries changes over time.

To address this limitation and enable the handling of moving boundaries, Eulerian equations must be reformulated to describe all physical quantities within the mesh coordinates. In this

mesh coordinate system, the domain remains fixed, and there's a direct mapping from the mesh coordinates to the current spatial configuration of the domain.

This transformation of physics equations onto a dynamically moving mesh leads to the development of the ALE method developed in Comsol (Ref. 9). Notably, if the mapping from mesh coordinates to spatial coordinates follows the material deformation, it reverts to a Lagrangian method. Conversely, when the mapping becomes an identity map, the ALE method becomes entirely Eulerian.

Consequently, the ALE method serves as an intermediate approach, combining the strengths of both Lagrangian and Eulerian methods. It facilitates the treatment of moving boundaries without necessitating the mesh to rigidly track material movement.

2.4 Mathematical modeling of the free surface generated by cladding and temperature field evolution

ALE method was used to generate deformed surfaces during DED AM. The addition of the successive layer during AM is modeled by moving (deformable) domain. The moving laser heat spot with the material addition is realized with boundary condition to the free surface of the deformable domain. The control of the surface height was regulated by the addition of the mass reflecting powder deposit velocity. The bottom surface was considered as a fixed one. All other surfaces of the deformable domain were under zeros velocity boundary condition. Such approach makes it possible to study in detail the melt pool depending on the process parameters. The simple geometry of the wall is considered to understand single bead wall formation when melt pool is of the size of the wall thickness. The melt pool is studied for different wall heights.

The characteristic examples of the deformable domains are presented in Fig. 2 where a 3-D contour plot of the temperature is presented at time 0.4 s. The scanning velocity is taken 1 cm/s and the laser power $q_0 = 1.25 \cdot 10^8 \text{ W/m}^2$ and laser spot diameter is 1 mm. The powder deposition is aggregated into the melt characterising the cladding process and is considered as a parameter v ranging from 1 to several mm/s which produces reasonable cladding domain heights.

In Fig. 2 the temperature distribution at 4 points on the top surface is presented on the right hand side. Since the wall height is not large the fast cool down process leads to a dwell time on the order of a tenth of a second. It is seen that temperature over several tenths of a second returns to the initial temperature. The temperature becomes the same as initial. For such a low wall height the dwell time is low. After the first layer is printed, the second one is following the same procedure as the first formed geometry as was used initially.

The characteristic temperature distribution in the wall emphasizing the melt pool domain is presented in Fig. 3. One can see the mushy zone details where the boundaries of the zone are at liquidus and solidus temperature. The taller wall domain simulation is presented in Fig. 3 where cross-section of the wall temperature distribution is presented by showing solid temperature, temperature in a mushy zone and in the melt pool separately.

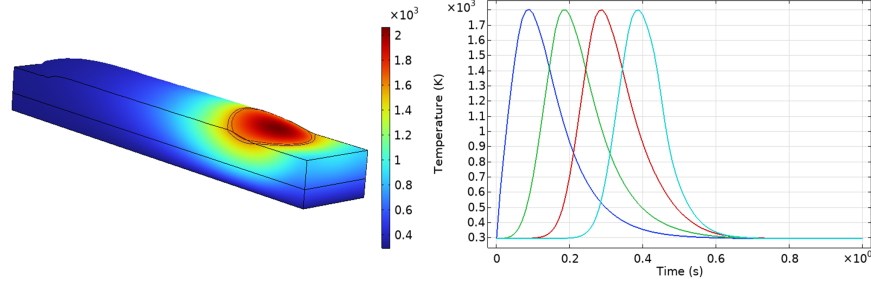


Figure 2.—The wall temperature for a short height model ($5\text{mm} \cdot 1\text{mm} \cdot 0.4\text{mm}$) – a), Surface temperature at $x = 0.2x_0 : 0.2x_0 : 0.8x_0$ dependent on time t , $x_0 = 5\text{mm}$ - is the length of the wall.

The dwell time of the taller wall increased substantially. For a wall of 2 mm high we obtain this value equal to several seconds as can be seen from the plot Fig. 4 – 6 where temperature history shows approaching 400K for time frames 1.5 s.

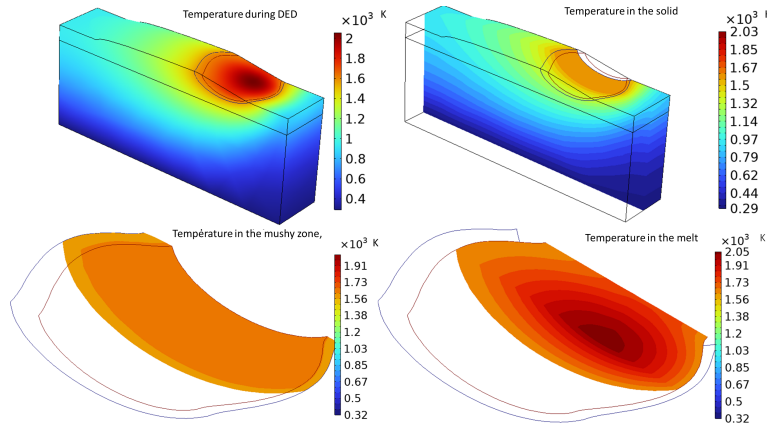


Figure 3.—Characteristic temperature distribution in the taller wall ($5\text{mm} \cdot 1\text{mm} \cdot 2\text{mm}$) for $t=0.4$ s. The temperature distribution in: a) wall during DED process – a), solid part of the wall – b) mushy zone – c) molten pool at time $t = 0.4\text{s}$, $q_0 = 1.7 \cdot 10^8 \text{W/m}^2$

It should be noted that temperatures showing heating, solidification, and cooling of INCONEL 625 are during deposition of one layer (Ref. 19) and this.

2.5 Temperature field evolution through the thickness at the cladding surface domain depending on the wall thickness

In this subsection a one bead wall for different thicknesses is analyzed. The 1 mm wall thickness is presented in Fig. 3 – 4. Throughout this report the thickness of the wall will be 1 mm if it is not otherwise specified. In this case increasing the height of the wall increases the dwell time as seen from Fig. 4 where dynamics of the three points through the thickness are shown. One point is on the nondeformable surface taken as initial wall surface, one is on the surface of the cladding domain and one is beneath the surface reflecting melt pool depth.

The wall height in Fig. 4 is 4 times larger than in Fig. 2 and the temperature relaxation grew to approximately 10 s. The melt pool cladding height for this simulation was 0.18 mm and the

melting region was at about the same scale since the lower point reached solidus. The top point curve in Fig. 4 appeared when the solid shape of the surface was formed.

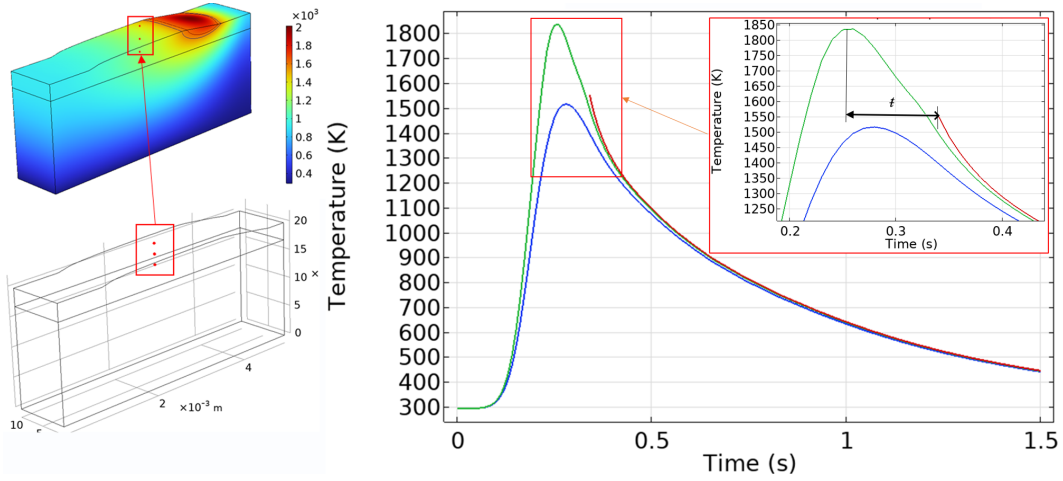


Figure 4.—Temperature evolution in the middle of the wall of 1 mm thickness for three points (see the plot on the left hand side) located on the clad surface, on the surface before cladding and beneath the surface characterising a melt pool depth.

The similar kinetics of the free surface formation is presented in Fig. 5 where the wall thickness is 2 mm and cladding height is about a quarter of mm. The melting depth is of the same order.

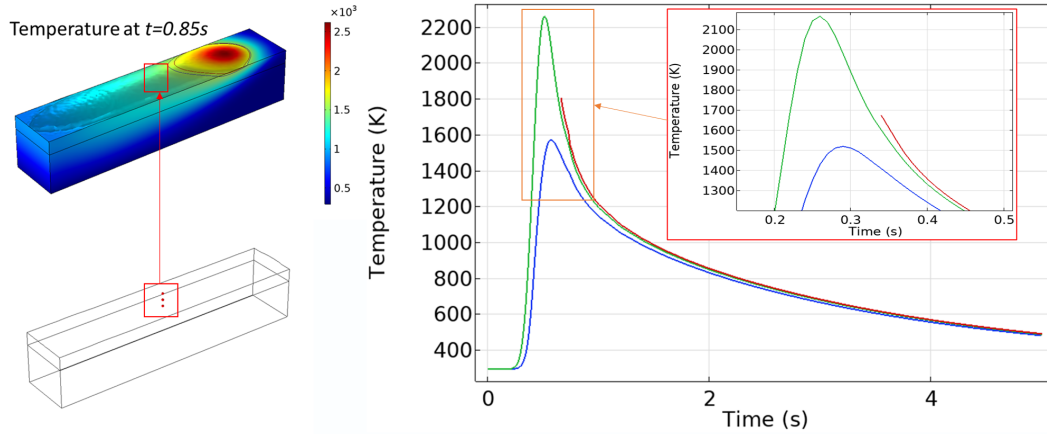


Figure 5.—Temperature evolution in the middle of the wall of 2 mm thickness for three points (see the plot on the left hand side) located on the clad surface, on the surface before cladding and beneath the surface characterising a melt pool depth.

For a 4 mm wall thickness (Fig. 6) an optimal cladding height is 0.5 mm and during cladding the laser practically remelts the same thickness of the layer which was built before.

It should be noted that during cladding mushy zone thickness increases. This is seen very pronounced for the thick wall (Fig. 6).

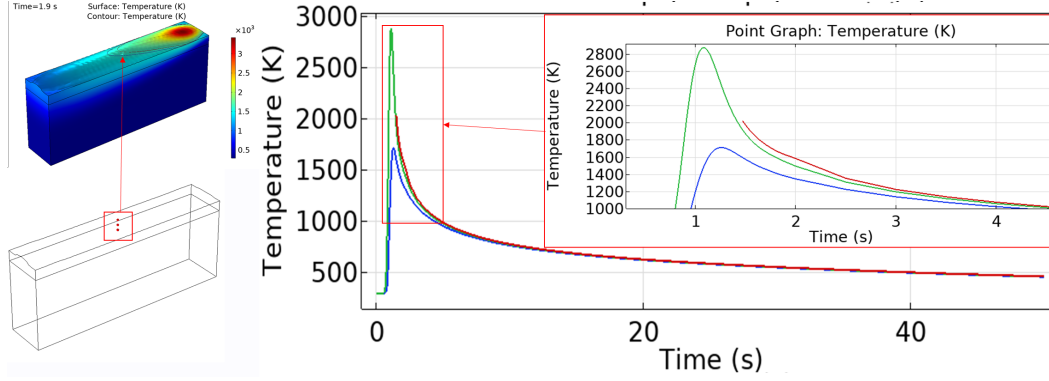


Figure 6.—Temperature evolution in the middle of the wall of 4 mm thickness for three points (see the plot on the left hand side) located on the clad surface, on the surface before cladding and beneath the surface characterising a melt pool depth.

The temperature dynamics as a function of temperature for 0.5 mm wall is presented in Fig. 7.

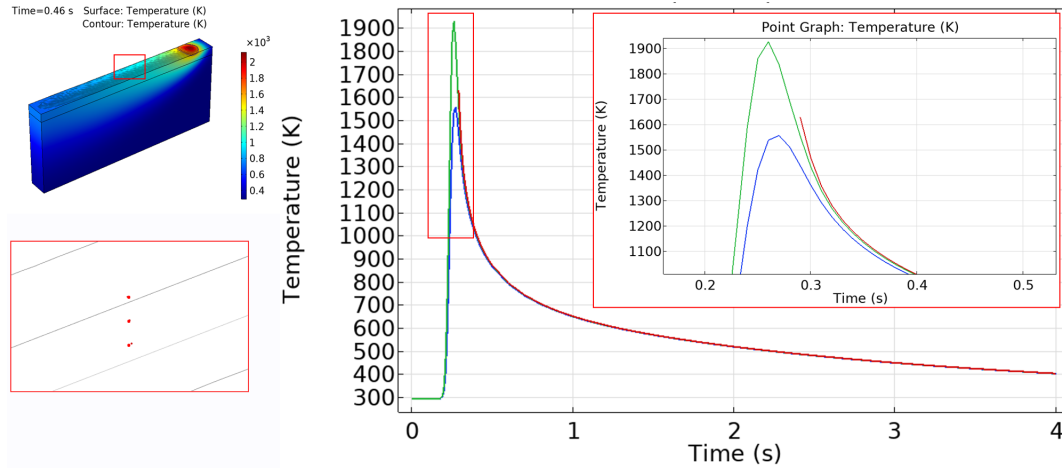


Figure 7.—Temperature evolution in the middle of the wall of 0.5 mm thickness for three points (see the plot on the left hand side) located on the clad surface, on the surface before cladding and beneath the surface characterising a melt pool depth.

From the temperature evolution of Fig. 4–7 one can see that as the thickness of the wall increases the higher the temperature of the cladding layer grows to manufacture a single bead wall. The linear dynamics of the maximum temperature (at the center of the wall) has a similar trend for all wall thicknesses. The melting of the wall surface and penetration of the melt beneath (points on the wall surface and below) are characterising the melt pool domain of the wall while the point on the clad surface is generated only after some time delay t needed for the addition of material to the top surface (Fig. 4). This delay is determined by the scanning speed and is of the order of the laser beam diameter (wall thickness) divided by scanning velocity. For Fig. 4 this delay time is about 0.1 s. At the same time the melting domain has a little delay in time when compared to the maximum temperature on the surface. The melt pool domain increases with thickness due to accumulation of more heat for the thicker one bead wall.

2.6 Cladding height as function of feeding rate velocity

For a 1 mm wall thickness the cladding height was studied as a function of the feeding speed v with constant laser scanning speed 1 cm/s. The results are presented in Fig. 8. The height changes from 80 μm at low feeding speed $v=1$ mm/s (Plot 1) until 550 μm at $v=6$ mm/s (Plot 6).

The linear plots of the maximum height (black line) is presented in Fig. 9. The larger speed v increases the height but at the same time the free surface shape became a little bit more irregular. The temperature plots 1–6 in the Fig. 8 show that the larger the cladding height becomes the higher is the temperature in the melt pool domain. As a result the cool down stage is larger as well leading to a larger dwell time. Analysis of the maximum temperature at the wall after starting cool down decreases as presented in Fig. 9. The maximum temperature is presented for two characteristic times $t=1$ s (red curve), and $t=2.5$ s (blue curve). At time $t=2.5$ s the temperature of the sample is below 400K even for the larger clad size (close to room temperature). At the same time for 1 s the temperature of the wall is large for a large cladding domain.

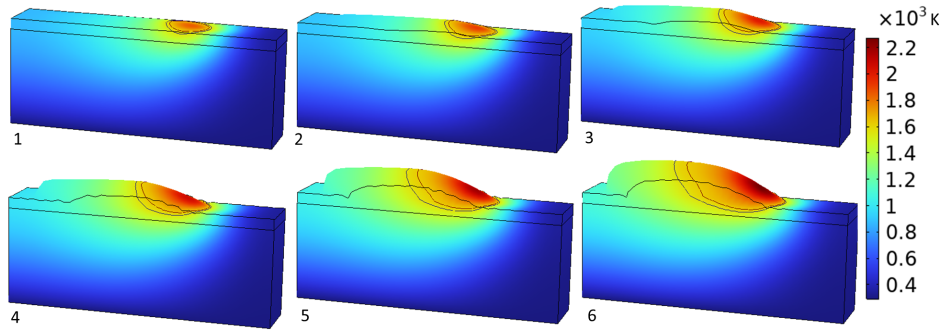


Figure 8.—The wall formation for different values of the cladding velocity: 1 – 1 mm/s, 2 – 2 mm/s, 3 – 3 mm/s, 4 – 4 mm/s, 5 – 5 mm/s, 6 – 6 mm/s. Surface temperature and shape deformation surface is presented at $t = 0.35\text{s}$.

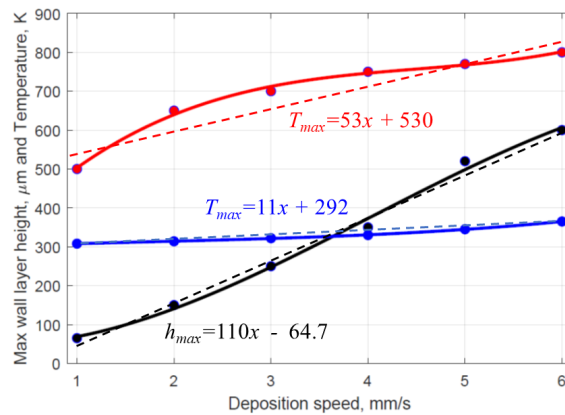


Figure 9.—Maximum height (black colour) as a function of deposition velocity v ($x[\text{mm/s}]$ on a plot) as well temperature during cool down stage at $t=1$ s (red line) and $t=2.5$ s (blue line). By dashed lines the linear regression line approximating data is presented for each set

3 Thermal Gradient Distributions and Cooling Rate

The developed approach enables the study of emerging gradients during the DED solidification process. These gradients in relation to wall heights outline the process's general characteristics which will be analyzed. Literature indicates that the solidification cooling rate and thermal gradients are important for microstructure control, as they significantly influence grain size, morphology, and the resulting mechanical properties of the build. This section will later demonstrate how these factors are influenced by process parameters and wall geometry, including thickness and height. Our objective is to identify general trends in these key parameters applicable to any experimental test.

The simplest approach is to analyze a specific thickness with semi-infinite length with a certain height, to establish reference values for these factors. In this case the Rosenthal's analytical solution for pure conduction problem (Ref. 20) could be used. However, the Rosenthal solution defines the steady state thermal field produced by a point heat source moving on the surface of a semi-infinite solid. In the real DED process we have a finite width with laser power localization on the order of the width. We will begin with smaller scales and observe the effects of increasing height and length. We exclude large (or infinite) width considerations, as our one-bead approach relies on wall side boundaries. This study aims to demonstrate that for each specific wall geometry, we can determine thermal gradients, cooling rates, and a process map to control microstructure. This includes examining the thermal gradient in the mushy zone, which influences solidification, flat front propagation instability, and morphology. Larger scale thermal gradients affecting residual stress will be studied in Section 6. Here, the focus is solely on thermal gradients and cooling rates in the mushy zone.

3.1 Melt pool shape and mushy zone temperature gradient distribution

The structure of the gradients evolves with increasing wall height, with typical examples shown in Figures 10 – 14. The typical thermal gradient distribution, $G = |\nabla T|$ increases for the largest value determined by the process parameters and laser beam location and then goes down. In the Figures 10 – 13 we can see the temperature distribution (dashed lines) and thermal gradients $G = |\nabla T|$ at the certain time increments $\Delta t = 0.1s$. The linear plots are taken along the dashed line with an arrow in the middle of the wall shown on the left. The temperature (dashed line) and thermal gradient G along this path are presented in the second plot. The temperature and gradient passes more or less have translational symmetry moving with the scanning speed. The third plot presents the distribution of the thermal gradient in the mushy zone.

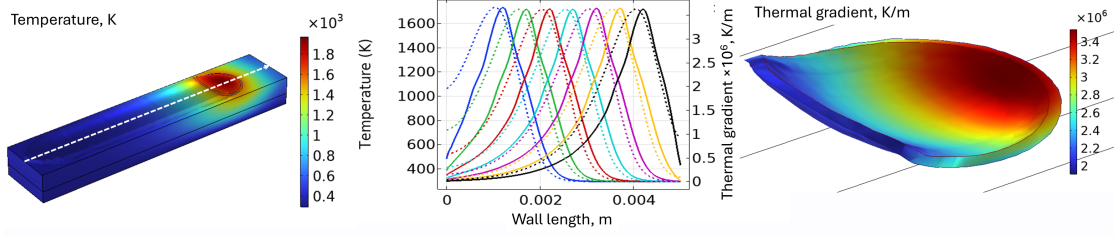


Figure 10.—Model of thin wall formation at low height ($h=0.5$ mm). Left: Temperature at $t=0.425$ s. Middle: Temperature and thermal gradient distributions along the top surface's central path at various times ($t=0.10$ s, 15 s, 20 s, 25 s, 30 s, 35 s, 40 s). Right: Thermal gradient magnitude in the mushy zone.

For the wall of a small height (Fig. 10) linear plots are monotonous for a cooling and heating domains. The linear plots varies based on DED wall processing parameters and wall height. For a low wall height (e.g., $h=0.5$ mm or less), the thermal gradient in the mushy zone is depicted in Figure 10. The temperature along a linear path at the sample's top surface is shown in the middle graph. Here, the temperature ranges from around 1800 K, with the thermal gradient magnitude peaking at 3.6×10^6 K/m, before decreasing as the melt pool tail cools. These correlated curves indicate that below the solidus temperature ($T=1573$ K), cooling occurs in the solid state. This trend suggests that at low wall heights, the main heat dissipation occurs through the substrate, which maintains a constant temperature around 300K, resulting in a thin mushy zone.

For a wall of 1 mm height the melt pool tail feature changes emerging from the path in the thermal gradient which is practically constant in mushy zone (Figure 11).

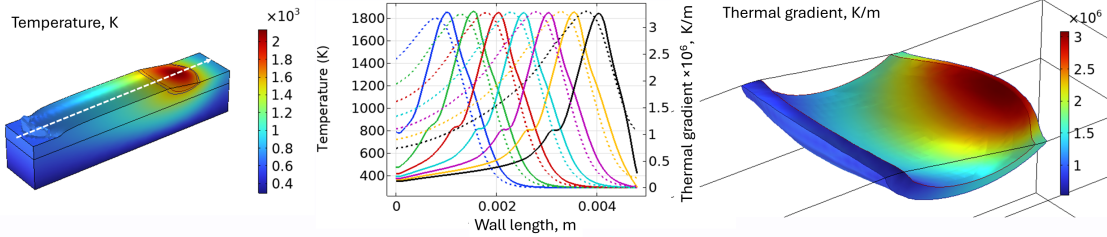


Figure 11.—Model of thin wall formation at low height ($h=1$ mm). Left: Temperature at $t=0.425$ s. Middle: Temperature and thermal gradient distributions along the top surface's central path at various times ($t=0.10$ s, 15 s, 20 s, 25 s, 30 s, 35 s, 40 s). Right: Thermal gradients in the mushy zone.

For a taller walls, temperature and thermal gradients are depicted in a set of Figures 12–13. The thermal gradient in mushy zone increases towards the melt pool surface. The mushy zone becomes thicker, and the thermal cooling gradient exhibits an N-shape like in Fig. 14. The drop in temperature at the solidus point reflects latent heat release during the liquid-to-solid phase transition. In contrast to Fig. 10, Fig. 12 – Fig. 14 show opposite trends in temperature and thermal gradient linear graphs. The thermal gradients display N-shaped tails, and the color variation through the mushy zone thickness is evident as it is seen in Figures 12–13. These figures illustrate similar temperature and thermal gradient distributions during DED processes along the central top surface

line at specific times. The left figure shows a contour plot of temperature distribution, with the mushy zone outlined and the central line indicating the measurement path. The right plots represent thermal gradients in the mushy zone. As the wall height increases, the mushy zone enlarges, and thermal gradient values slightly decrease at the mushy zone's tail. The gradient becomes non-linear with an N-shaped curve at the solidus surface. These middle plots correlate with the melt pool thermal gradient distribution. The area near the solidus surface is brighter, indicating latent heat release and heat dissipation from the melt pool's solidus surfaces. This phenomenon, more pronounced in taller walls, leads to larger melt pool dimensions and mushy zones due to insufficient heat dissipation to the substrate and preheating of the wall volume.

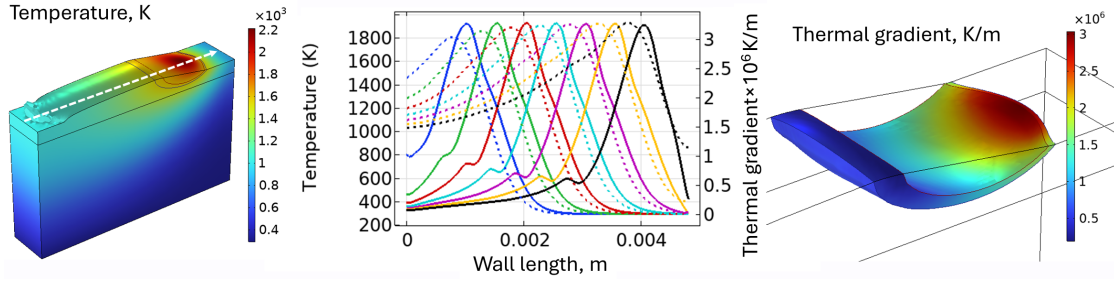


Figure 12.—Model of thin wall formation at low height ($h=3$ mm). Left: Temperature at $t=0.425$ s. Middle: Temperature and thermal gradient distributions along the top surface's central path at various times ($t=0.10$ s, 15 s, 20 s, 25 s, 30 s, 35 s, 40 s). Right: Thermal gradients in the mushy zone.

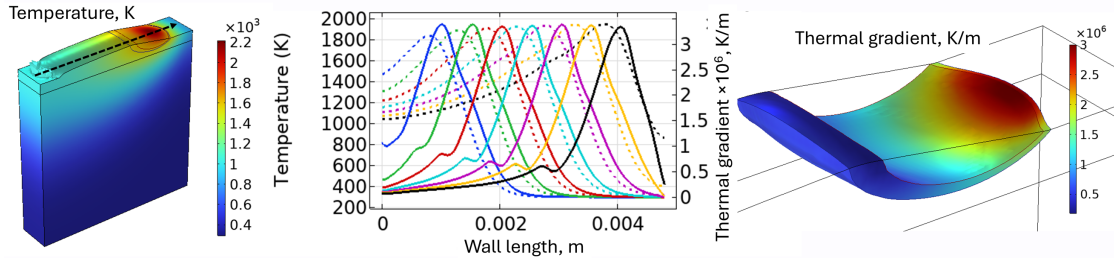


Figure 13.—Model of thin wall formation at low height ($h=5$ mm). Left: Temperature at $t=0.425$ s. Middle: Temperature and thermal gradient distributions along the top surface's central path at various times ($t=0.10$ s, 15 s, 20 s, 25 s, 30 s, 35 s, 40 s). Right: Thermal gradients in the mushy zone.

The negative slope of the thermal gradients in the tail of the melt pool is very important since it determines the local undercooling controlling the microstructure formation. By adjusting the dwell time, we can model wall manufacturing by varying the height. Results in Figures 10–13 show similarities between low and tall wall manufacturing, with distinct features emerging from changes in wall height. The key findings relate to melt pool size and thermal gradients. To maintain a single bead wall structure, it's necessary to reduce laser power. Keeping the same power enlarges the melt pool, significantly affecting the cooling rate. Studying the time–temperature profile is important, especially for intrinsic heat treatment (IHT) (Ref. 21). The temperature and duration

of IHT depend on the thermal history of a specific location, which is influenced by the balance of heat input and loss. Maintaining this balance without increasing temperature allows IHT to enhance the properties of the manufactured wall. Standard cladding processes with short dwell times, where temperature rises, are discussed latter on.

For better understanding thermal parameters relationships the middle cross-section of the one bead wall during cladding layer is presented in the Fig. 14 a) and b) where some characteristic feature of the temperature and thermal gradient are presented. In this report the magnitude is used for analysis, that is why the real gradient and gradient magnitude are compared in Fig a) and b). On both plots the laser spot moves from the left to the right. The top contour plot presents the temperature at time $t=0.35$ s. The plot below the temperature distribution shows the real thermal gradient – a) and gradient magnitude – b).

The linear plot graphs determine the temperature along the sample on the top surface and are correlated with the contour plots. One can see that when the heat source is moving from the left to the right, the temperature (blue line) increases up to a certain values greater than melting temperature and then goes down (it is analysed from the right to the left). Where the temperature is greater than phase transition one can see the melt pool on the top plot. In the mushy zone characterised by two temperatures T_{solid} and T_{liquid} the phase field transition has taken place. The maximum temperature is sqewed to the right characterising larger gradients for heating than for cooling. The negative value of the gradient in the left plot reflects heating the wall by laser and cladding material, and positive one – the cooling material during solidification. The left plot showing gradient magnitude and its slope is negative for heating and positive for cooling. The vertical lines emphasize characteristic features of the DED process. One can see that maximum gradient is located in the position of the solidus line (vertical line 4). The maximum temperature is in a melt pool close to the front of the melting boundary (vertical line 3). The two next vertical lines – 2 and 1 reflect cooling features – liquidus temperature position is characterised by line 2, and the solidus temperature by line 1.

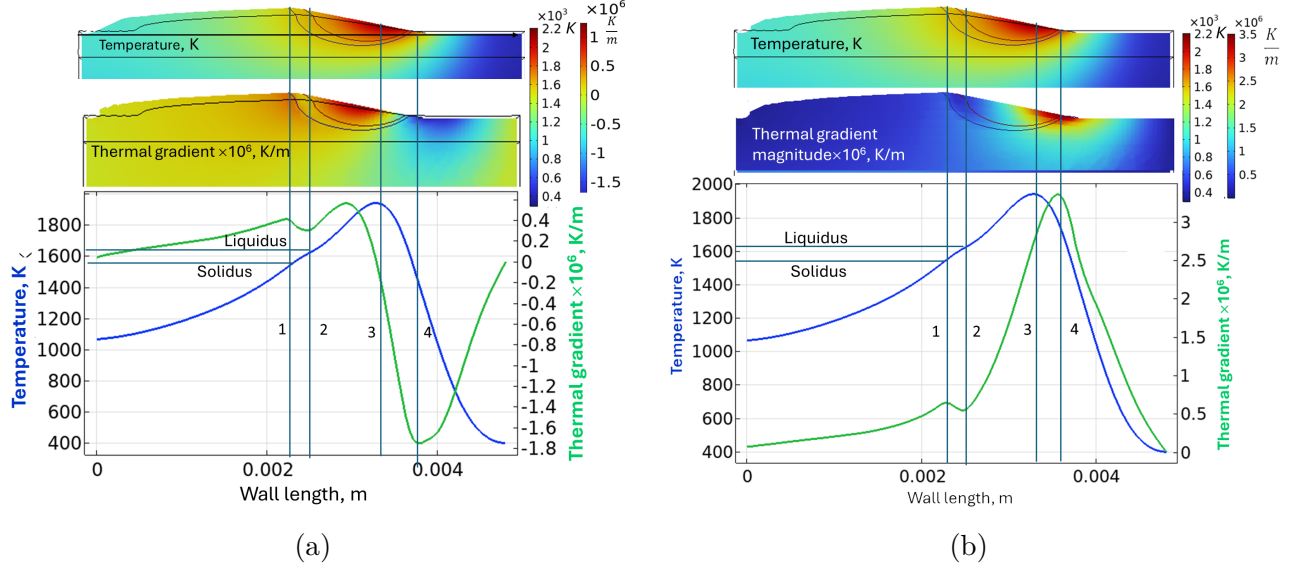


Figure 14.—The cross-section of the wall along the propagation direction used for detailed explanation of the characteristic features of the melt pool: first layer is temperature, second one is thermal gradient and gradient magnitude, third one is a linear plot of the temperature and gradients along the path on the top of the wall.

3.2 Solidification velocity and cooling rate for moving mushy zone

The second critical parameter in determining the scale of the final microstructure is the cooling rate (CR) – ϵ . The melt pool shape and mushy zone are influenced by various processing parameters and material properties. The cooling rate in the sample, $-dT/dt$, can be easily calculated as the entire temperature field over time can be analyzed. The tail dynamics is under investigation here, particularly when the tail of the melt pool dissipates heat quickly. The cooling rate in the melt pool and mushy zone is vital for the stability of the solidification front and ultimately affects the morphology of the structure.

3.2.1 Solidification velocity

The solidification rate (R) is determined by the laser scanning speed v and the angle α between the scanning direction and normal to the melt pool's surface, as expressed by the equation (Ref. 22, 23):

$$R = V \cos(\alpha), \quad (7)$$

where the solidification rate R is the velocity of the melt pool boundary normal to the melt pool surface and is determined by the normal gradient $G_n = (\nabla T)_n$, $|G_n| = (|G_x|^2 + |G_y|^2 + |G_z|^2)^{1/2}$. The laser scanning pattern in the x-direction is determined by $\cos(\alpha) = |G_x|/|G_n|$.

From equation (7), it is evident that higher scanning speed typically results in greater growth rate, and the smaller the angle, the higher the solidification rate. The product of the temperature gradient G and the solidification rate R determines the cooling rate ϵ . The interplay between R and G significantly impacts the resulting microstructure during solidification. The larger the cooling

rate, the smaller the dimensions of the microstructure. We will analyze this phenomenon based on a solid theoretical background developed in the theory of crystallization (see the next Section).

As in a previous section a thin wall (thickness 1 mm) was considered for thermal and shape modeling (Fig. 15), where temperature and cooling rate along the Z-path are presented for several time frames. One can see that three temperatures are at the frames when the laser spot passes the center point and three others are after passing the central point when the temperature propagates to the base. The cooling rate at the same time frames is negative (blue, green, and red in the middle curves), meaning heating of the sample, and then the sample starts to cool down.

The temperature gradient magnitude are presented in Figures 10–13 for the path along the x axes. Here the same XZ-plane is considered and path is located in the middle of the sample. One can see that the largest heating rate is in the melt pool domain and in front of it, while the largest cooling rate might be at the solidification domain determined by a mushy zone. Since the velocity of the laser in this simulation is 0.01 m/s, the heating-cooling rates must be scaled by a factor of 0.01, as shown in the vertical axis on the right-hand side.

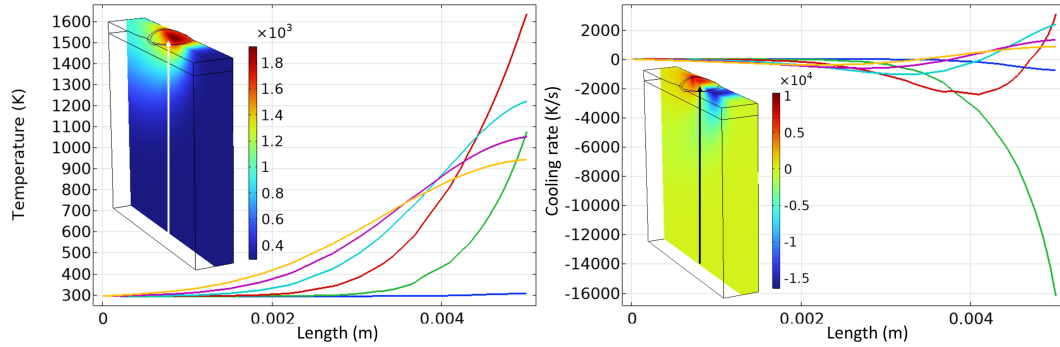


Figure 15.—The temperature along the vertical path at the center of the wall as shown on the insert to the linear plot – left, and cooling rates along the same path – right. The middle plane XZ of the thin one-bead wall is presented for temperature and cooling rates correspondingly. The time frames are 0.1 s – blue, 0.2 s – green, 0.3 s – red, 0.4 s – blue, 0.5 s – violet, 0.6 s – brown.

3.2.2 Cooling rate in mushy zone

The general view of the thermal gradient and cooling rate for the thin wall sample during DED manufacturing is presented in Fig. 16 – 19 for a certain time $t=0.3$ s, where maximum values are located in the region of the melt pool, mushy zone and nearby. That is why comparison of these values is presented in the mushy zone domain solely. These contour plots look similarly but are scaled by solidification velocity. To single out a more detailed characteristic of the cooling rate mushy zone, the cooling rate is presented in Fig. 17 where a continuous colour plot is substituted by a discrete one to emphasize the difference of the cooling rate patterns on the liquidus and solidus surfaces.

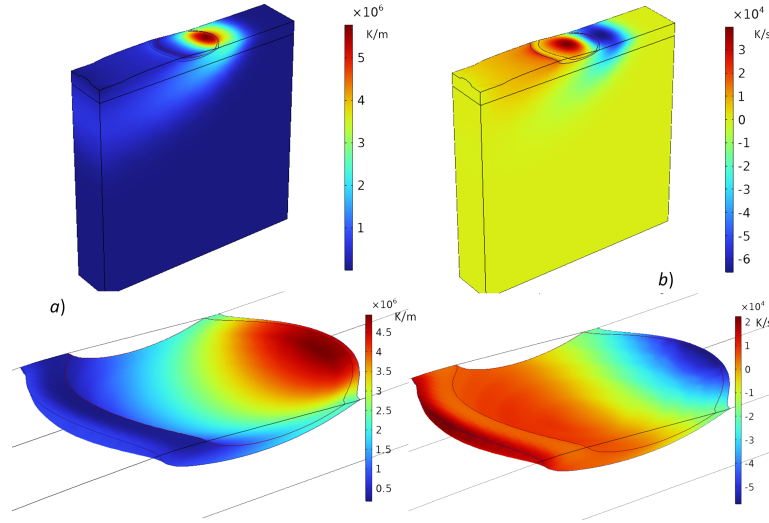


Figure 16.—Thermal gradient magnitude – a) and cooling rate – b) for a thin wall. The corresponding variable distributions in the mushy zone is seen in the zoomed melt pool domain.

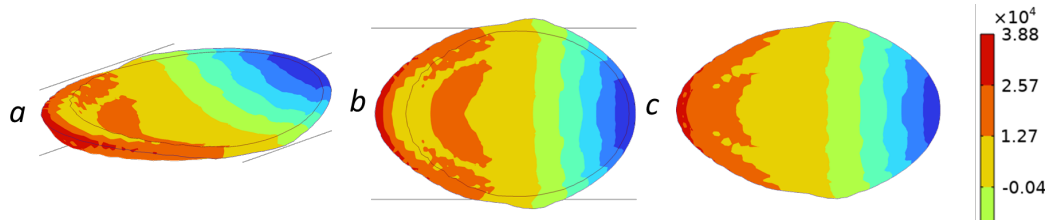


Figure 17.—Mushy zone cooling rate distribution for the scanning velocity 3 cm/s: isometric view – a), view from the top – b), and downside of the mushy zone – c).

The cross-section of the melt pool mushy zone is presented in Fig. 18. This plot contains interconnected mushy zone parameters. The temperature through the mushy zone changes from the liquidus to the solidus. The thermal gradient is largest during the melting process and smallest during cooling. The gradient is larger at the solidus position, as discussed earlier. The solidification velocity is largest at the tail and negative for the melting surface, as the direction of the normal to the surface is opposite to the scanning velocity. The cooling rate (ϵ) is maximum on the tail (solidus surface) line and decreases, having a minimum at the point where the solidification velocity changes sign.

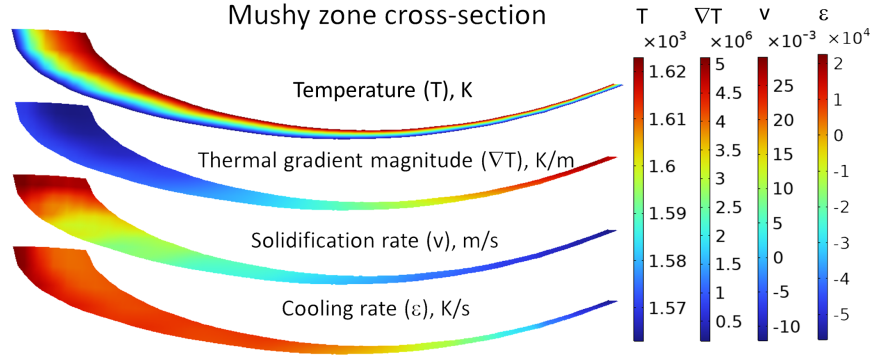


Figure 18.—The temperature distribution across the mushy zone – top, The thermal gradient and solidification velocity in the middle, and cooling rate – bottom plot for the middle plane XZ of the thin wall one-bead formation.

It is possible to reproduce an analytical model of the melt pool Fig. 19 extracting data from the mushy zone plot. On the right hand side as an example one can see solidification velocity as a function of the melt pool position.

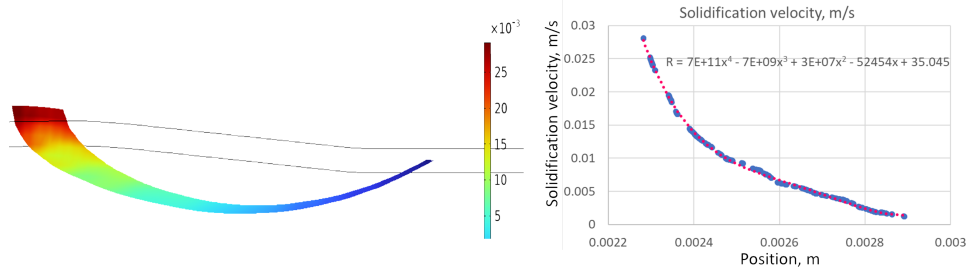


Figure 19.—Contour plot of the solidification rate in mushy zone for scanning velocity 3 cm/c – right and solidus line boundary with approximated equation of the melt pool.

Some characteristic features of the geometric parameters during cladding, the linear plots for solidus boundary are presented for scanning velocity 1 cm/s as an example (Fig. 20). One can see that melt pool length is about 1 mm and the solidification rate is presented for each point of the solidus position. Solidification velocity (top left plot) is maximum close to the top surface approaching scanning velocity. At the bottom of the melt pool it became zero, increasing x coordinates shows that it changes sign characterizing the melting process. The maximum melting velocity is about 50 percent less than scanning one. The top right hand side plot shows the solidus z-position depending on z coordinate. The initial position of the wall was taken as 5 mm in height. The melt pool depth is 0.1 mm which can be seen from the plot where z=4.9 mm corresponds to the solidus line. By increasing z again we have two branches: solidification and melting one. One can see that the thickness of the cladding layer is 0.2 mm and total melted domain is about 0.3 mm in thickness.

The value of the thermal gradient (x axis) can be seen from bottom left hand-side plot and it changes from 0.8e6 K/m at the cladding surface until 1.5e6 K/m at the melt pool depth. The cooling rate (x axis)–bottom right hand side plot increases from zero at the bottom of the melt

pool depth till 7.5×10^3 K/s near the top of the cladding surface. Heating rate in front of the laser beam changes from 1.25×10^4 K/s till zero at the bottom of the melt pool.

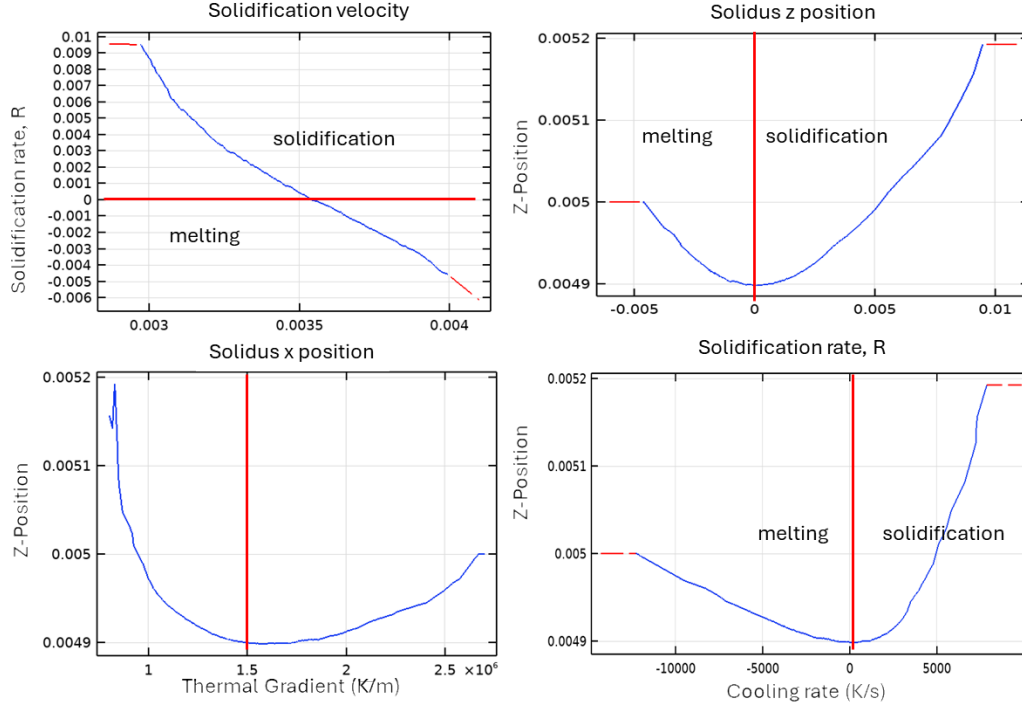


Figure 20.—Solidification rate as a function of the x-coordinate (top left), z - Position of the solidus boundary as a function of solidification rate (top right), z - position as a function of thermal gradient and cooling rate (bottom plots). The data are extracted from middle plane XZ of the thin wall.

3.3 Cooling rates and gradients change with respect to wall thickness

The analysis of how cooling rates vary with wall thickness is presented below. This variation directly influences the microstructural characteristics of single bead walls. We aim to compare cooling rates in walls of different thicknesses, as illustrated in Figures 21 to 24. These figures present a comprehensive view: the first graph shows the wall's general structure, the second details cooling rates, and the third illustrates thermal gradients in the mushy zone.

A key aspect of our analysis is the stationary temperature condition in all walls, attributable to their significant height and prolonged dwell time. We begin by exploring the melt pool processes at the solidification front, focusing on solidification along the rear boundary of the moving melt pool. This focus is very important as the microstructures on the tail side are shaped by the local temperature gradient (G) and solidification velocity (R), with their product (GR) determining the cooling rate, as discussed in the previous subsection.

For our simulations, we maintained a constant scanning speed of 1 cm/s. We observed that melt pools enlarge with increased wall thickness, which also significantly extends the dwell time. Consequently, both cooling rates and thermal gradients diminish as wall thickness increases (Fig. 21 – 24).

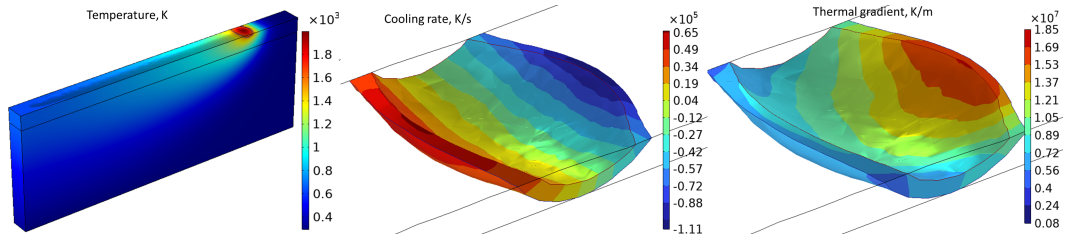


Figure 21.—Melt pool analysis for wall thickness 150 um (Ref. 24), temperature, cooling rate and thermal gradient, correspondingly

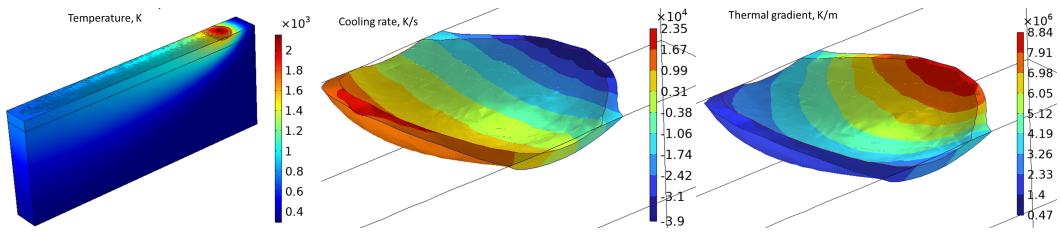


Figure 22.—Melt pool analysis for 500 um wall thickness, temperature, cooling rate and thermal gradient in a row

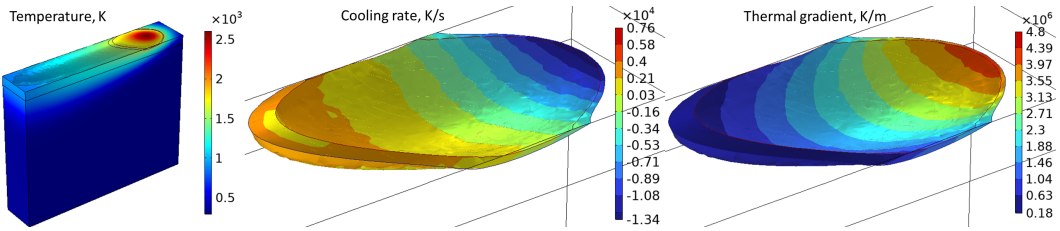


Figure 23.—Melt pool analysis for wall thickness 2mm, temperature, cooling rate and thermal gradient in a row

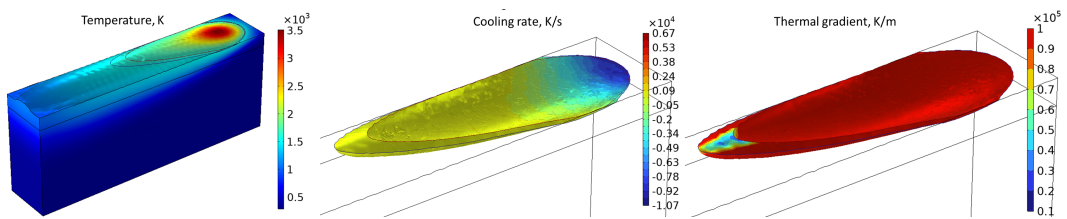


Figure 24.—Melt pool analysis for wall thickness 4 mm, temperature, cooling rate and thermal gradient in a row

The considered model is applied to DED process but the same approach might be developed to PBF AM. In last case case the scales of the temperature distributions will be different reflecting much larger thermal gradients and cooling rates (Ref. 25).

3.4 Cooling rates during the cool down stage

In this section, the cooling down stage is investigated with respect to wall thickness. The accumulated heat during AM is influenced by various factors, including dwell time and wall thickness. We focus on cooling in the temperature range below the solidification frame, which does not alter the microstructure formed by the dynamics of the melt pool. However, if the solid material undergoes phase transformations, the cooling rate, varying with wall thickness, can modify the microstructure.

The cooling rate is influenced by the material's thermophysical properties, the geometry of the structure, and the heat transfer coefficient to the environment. We calculated cooling rates for each wall thickness by deriving the transient temperature plots (see insert and main plot) to obtain the rate of temperature change (dT/dt) as depicted in Figure 4 – 7. Our findings indicate that the cooling rate is highest at the onset of cooling and gradually reduces to zero as the wall temperature equilibrates with the environment. Thinner walls exhibit higher cooling rates, decreasing as the wall thickens due to their larger heat capacity, which requires more time to dissipate energy.

The cooling process is also significantly affected by the convection coefficient, set at $10 \text{ W/m}^2\text{K}$ in our simulations. The sink and baseplate were maintained at 300K . With a short dwell time (1-2 s) for a tall wall (approximately 5 mm), there's notable heat accumulation during printing. The final cool down rates, shown in Figure 25, start from around $1\text{e}4 \text{ K/s}$ and decrease exponentially with increasing dwell time. Each wall thickness corresponds to a specific cooling time, revealing that thinner walls may experience higher cooling rates.

We also established that the temperature gradient G , and the melt pool shape velocity R depend on wall thickness under the same laser beam parameters. Consequently, the trailing edge of the melt pool (as seen in the walls Figures 21 to 24) exhibits varying cooling rates.

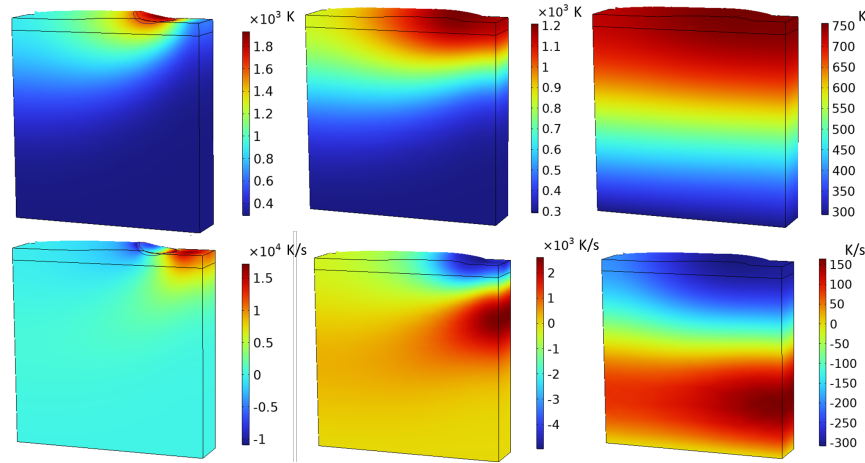


Figure 25.—The temperature distribution (T) – first row and cooling rate (K/s) – second row for wall height 5 mm at $t=0.4 \text{ s}$, $t=0.5 \text{ s}$, $t=1.0 \text{ s}$ correspondingly.

The cool down rates can be estimated for a certain points on a top wall surface as presented in Fig. 26, One can see that sharp change of the cooling rates at the time when melt pool region passes this point. This change in cooling rate is localized by a small time interval behind this interval cooling rates are sufficiently small characterising slow cooling down rate of the wall.

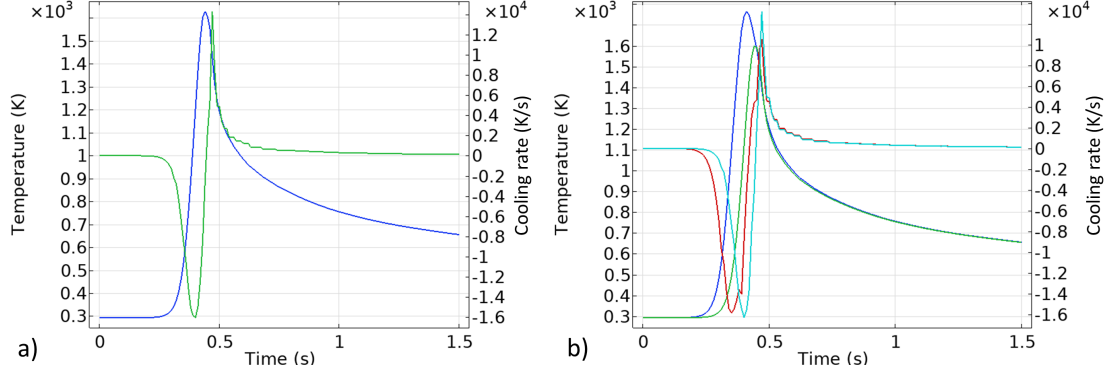


Figure 26.—The time temperature distribution at the middle of the top surface point $x=4.5$ mm and corresponding cooling rate – a), and the same distribution for a central and side points for $x=4$ mm.

3.5 Difference in cooling rates for several deposited layers

The melt pool of three successive layers is presented in the Fig. 27. The melt pool increases in size for each successive layer. In this simulation the temperature distribution was taken from the previous layer and as a result heat accumulation leads to substantial increase of the melt pool domain singled out by two curves (solidus and liquidus one).

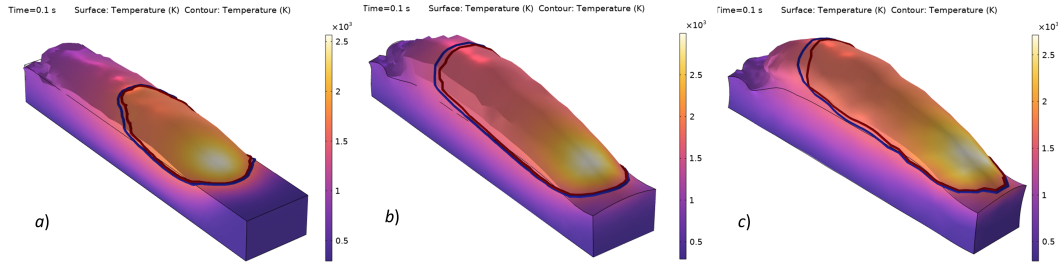


Figure 27.—Melt pool dimensions for a first layer – a), second – b) and the third one – c).

The shape of the multilayer formation is presented in Fig. 28 where first row reflects cladding with smaller scanning velocity and for the second layer scanning velocity is 3 times larger. As a result, for such small sample the layers are more inhomogeneous. The matter is that for the larger scanning velocity we need a longer wall to perform quasi-stationary cladding. In the figure for a short time we add cladding and then should stop it stabilize cladding on the boundary of the sample.

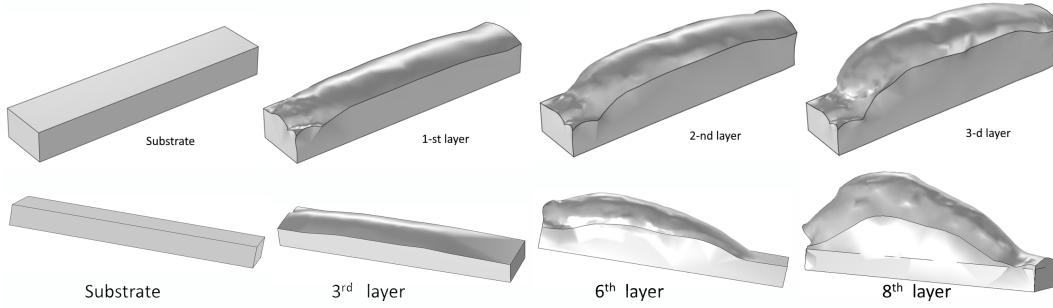


Figure 28.—Thin wall formation model: The initial slab used for DED modeling, the first layer shape often cladding, second and third one for the cladding velocity 1 cm/s – first row, and similar approach for 8th layers for cladding velocity 30 mm/s - second row.

The detailed study of the 4 layer cladding as an example is presented in Fig. 29. The small dwell time leads to overheating the manufactured sample. As an example four layer formation is presented in Fig. 29 where for the small dwell time we have a temperature distribution after build-up. The first layer is printed at substrate temperature 300 K, the second layer has temperature distribution with a maximum about 500 K, for the second one the temperature reaches about 900 K, and for the third one the temperature is approximately 1100 K. These results were used for the cooling rate simulation presented in Fig. 30.

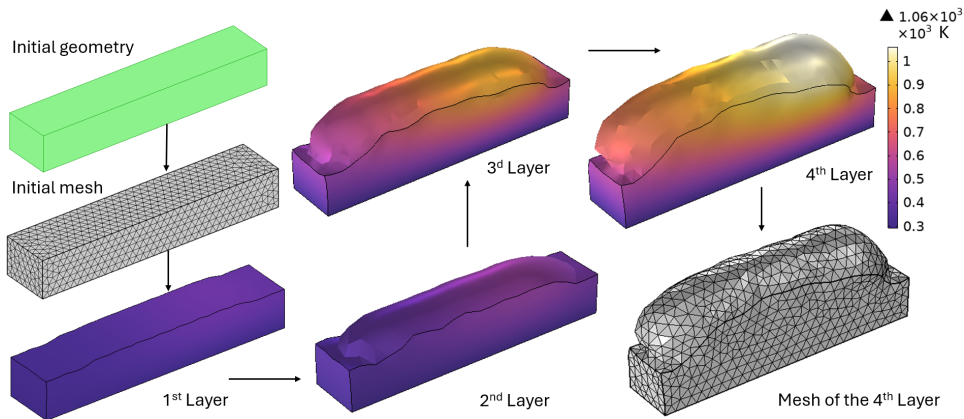


Figure 29.—Thin wall formation model for the first 4 layers: The initial slab used for DED modeling with initial mesh, then first, second, third and forth layer shapes with temperature distribution for a small dwell time.

The following set of mushy zone plots (Figures 30) presents simulation results for four consecutive layers in an additive manufacturing process. The initial conditions for each layer differ: the first layer starts at room temperature, while the subsequent layers begin with the temperature distribution from the previous layer (see Fig. 29). As a result the last 4th layer plot has the highest temperature after build up.

These simulations reveal a notable pattern: the cooling rates for all three melt pools, initially set at 300 K, are higher compared to those starting with a temperature distribution carried over from the previous layer. This finding underscores that the cooling rate decreases as the dwell time

between layers is reduced, leading to a corresponding increase in the scale of the primary dendrite arm spacing (PDAS (Ref. 26), see details in the next section).

It's important to point out that in larger structures with substantial dwell times—allowing cooling to room temperature—the cooling rate becomes nearly uniform across each layer. Consequently, the PDAS distribution will likely exhibit a consistent scale across the structure.

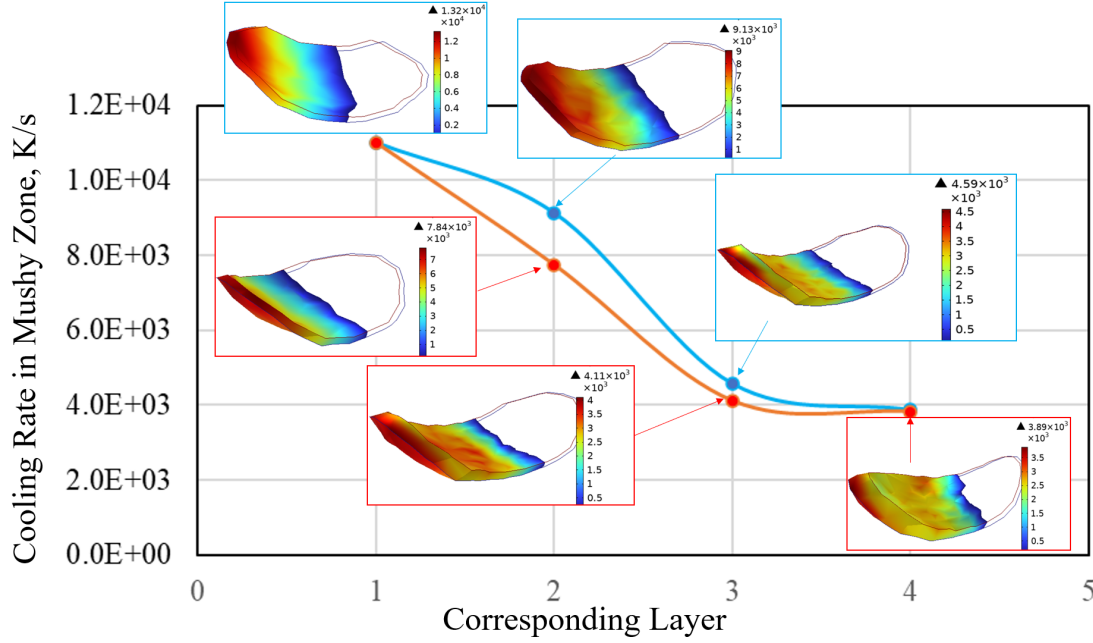


Figure 30.—The cooling rate in mushy zone for 4 layers, presented in Fig. 29 with small dwell time.

The conclusion is drawn here reflects that the larger is initial temperature for the layer cladding the smaller is cooling rate at the melt pool tail as presented in the Figure 30.

4 Microstructure Consideration

Understanding the formation of cellular and dendritic structures in DED manufacturing is pivotal, significantly impacting mechanical and structural properties, and ultimately, part performance. This section explores the characteristic features of these structures, drawing on previous studies of non-equilibrium solidification in alloys. Key parameters like thermal gradient, solidification velocity, and cooling rate, discussed earlier, are key in predicting microstructural characteristics of clad materials and grain structure.

Dendritic structure formation during solidification processes is triggered by undercooling, where a melt is cooled below its equilibrium freezing point before solidification. Undercooling can occur due to impurities or specific physical conditions at the temperature below solidification. It promotes dendrite formation by creating favorable conditions for nucleation and growth. Nucleation sites form randomly within the melt during undercooling, serving as seeds for dendritic growth. Thus, undercooling significantly influences nucleation and growth kinetics, ultimately shaping the

solidified material's final morphology. The typical dendrite structure is schematically presented in Fig. 31. In metals, such dendritic structures form a microstructure of a certain scale known as primary dendrite arm spacing (PDAS), the size of which depends on the cooling rate.

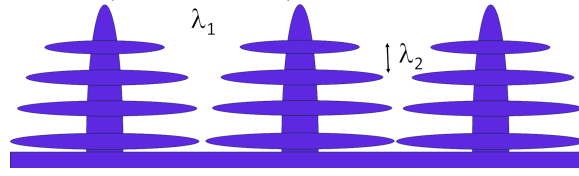


Figure 31.—Sketch of the PDAS structures (Ref. 26). Violet shape shows typical morphology of the solidification front.

4.1 The primary dendrite arm apacing

Dendritic structures form within the melt pool under local undercooling conditions, typically arising from concentration redistribution in metal alloys. This phenomenon leads to the emergence of nonhomogeneous structures at solid-liquid interfaces, triggering a bifurcation and entering a non-linear stage characterized by a specific growth rate known as the Mullins-Sekerka instability (Ref. 27, 28). During this phase, primary dendritic arm spacing develops at a nearly constant velocity, creating a periodic morphology in the solid state. In materials like INCONEL 625, this nonlinear solidification process involves niobium (Nb) rejection near dendritic tips, enriching interdendritic regions and facilitating secondary dendritic growth (Ref. 26, 29? , 30).

Primary dendrite arm spacing (λ_1) is an important parameter in microstructure formation directly linked to the cooling rate. It is influenced by various physical processes in DED, such as melt pool formation and interlayer dwell time. Our simulations illustrate how the molten pool's shape and associated microstructure evolves with changes in scanning speed. Increased scanning speed reduces both linear laser energy and powder feed rate, resulting in a smaller molten pool.

The primary dendrite arm spacing, λ_1 , can be estimated using the Kurz-Fisher model, which relies on the principle of constitutional supercooling. This model highlights the heavy dependence of alloy solidification microstructure on process parameters like local thermal gradient (G) and solidification rate (R) (Ref. 25, 30–33).

$$\lambda_1 = AG^{-a}R^{-b}, \quad (8)$$

where

$$A = 4.3\Delta T^{0.5} \left(\frac{D_L \Gamma}{\Delta T_0 k} \right)^{0.25}, \quad (9)$$

or

$$A = 4.3(\Delta T_0 D_L \Gamma / k)^{0.25}, \quad (10)$$

Here, D_L is the diffusion coefficient in liquid, ΔT_n is the non-equilibrium solidification range, ΔT_0 is the equilibrium solidification range, Γ is the Gibbs-Thomson coefficient, R is the solidification rate, and G is the thermal gradient.

The PDAS plot for typical parameters in DED manufacturing of INCONEL 625 is presented in Figure 32 a. This plot illustrates how PDAS varies with different manufacturing conditions, offering insights into the microstructure of INCONEL 625 as it undergoes the DED process.

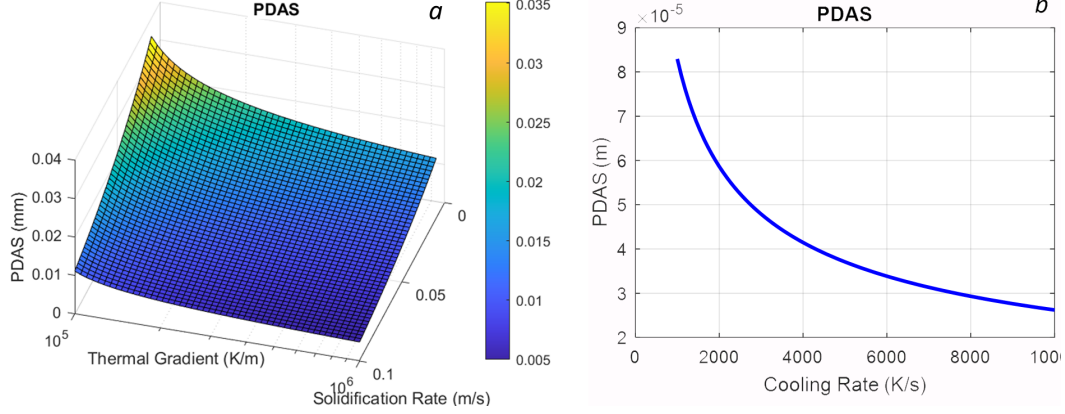


Figure 32.—The PDAS dependance on the solidification velocity and thermal gradient – a) and PDAS dependance on cooling rate – b). The blue line is phenomenological curve (Ref. 30, 31, 34)

A simple relationship (as per Equation (8)) provides a quantitative method to discern microstructural differences under different thermal conditions. The relationship between PDAS and cooling rate is well-established in literature. Figure 26 illustrates the dependency of cooling rate on wall thickness, where the red line approximates the trend based on simulations of melt pool dynamics. For a thin wall (1 mm thickness), the cooling rate near the center plane is about 5×10^3 K/s, correlating with a PDAS value of approximately $5 \mu\text{m}$.

In the context of DED manufacturing, the relationship between the thermal gradient (G), solidification velocity (R), and cooling rate (ϵ) determines the morphology of the microstructure. The product of the thermal gradient and velocity, GR , is directly related to the cooling rate as follows:

$$\epsilon = GR, \quad (11)$$

where ϵ is the cooling rate in K/s. This relationship indicates that an increase in the thermal gradient, coupled with solidification velocity, enhances the cooling rate, thereby reducing the period of the morphological structures.

A simplified relation for estimating the PDAS can be utilized (Ref. 34, 35):

$$PDAS = 80 \cdot \epsilon^{-1/3}, \quad (12)$$

which suggests that dendrite spacing decreases as the cooling rate increases. This equation provides a more straightforward approach for estimating PDAS, as shown in Figure 32 b).

Similarly, the Secondary Dendritic Arm Spacing (λ_2) is influenced by the cooling rate (CR) (Ref. 36–38):

$$\lambda_2 = 25 \cdot \epsilon^{-0.28}. \quad (13)$$

This relationship underscores that λ_2 also varies depending on the cooling rate.

For fine columnar dendritic structures, the yield strength (σ_Y) can be correlated with λ_2 using a Hall-Petch-like equation (Ref. 39, 40):

$$\sigma_Y = \sigma_0 + K \cdot \lambda_2^{-0.5}, \quad (14)$$

where σ_Y is the yield strength in MPa, and σ_0 and K are material-specific constants. For INCONEL 625, σ_0 is 108 MPa, and K is 1340 MPa. This equation links the secondary dendritic arm spacing

to the strength properties of manufactured INCONEL 625. However, it's noted that the predicted values according to this equation are typically less than the experimental data.

In contrast, other studies (cited as (Ref. 7, 41)) report a value of K as $750 \text{ MPa}/\mu^{1/2}$ and σ_0 as 691 MPa , which is equivalent to the yield strength of the solid material. Using these values, the equation over-predicts the experimental results. This variation in the constants used in the Hall-Petch-like equation highlights the importance of accurately determining material-specific parameters for precise predictions of mechanical properties in DED manufactured materials.

4.2 Microstructure evolution of solidified laser cladding layer

If the ratio G/R decreases then the solidification front changes from planar to cellular growth, next from columnar dendritic to equiaxed dendritic growth (Fig. 33) (Ref. 7). At the same time if cooling rate ratio ϵ decreases the average size of the microstructures become smaller. The linear graphs on figure a correspond to the border of different regimes which characterized by different slopes G/R , and red lines equal to $\epsilon_1 < \epsilon_1$ correspond to different cooling rates.

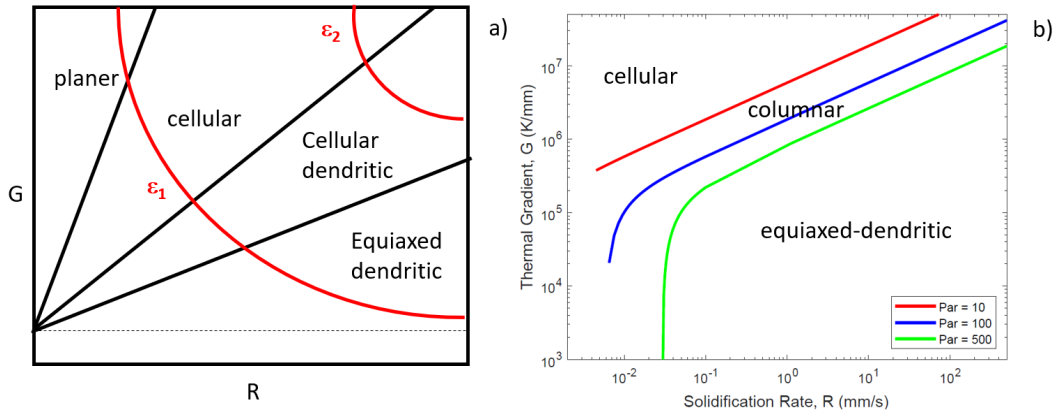


Figure 33.—Schematic diagram of the possible modes of microstructure formation – a), and columnar to equiaxed transition (CET) diagram (general view) –b).

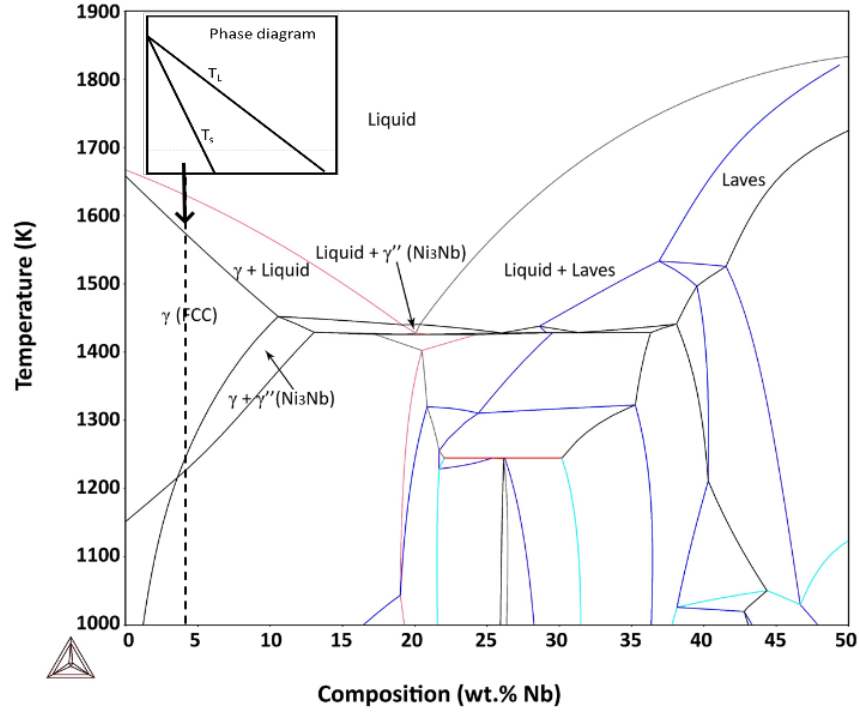


Figure 34.—Phase diagram for INCONEL625 calculated via the Thermo-Calc software (Ref. 42, 43).

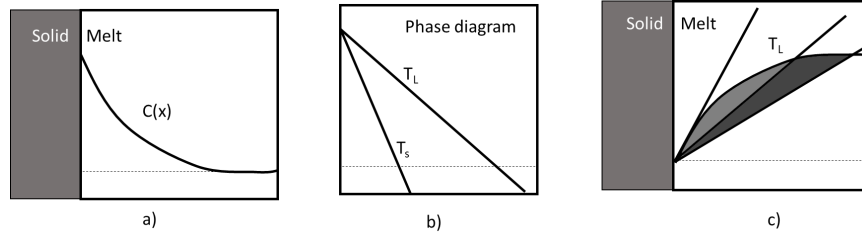


Figure 35.—Constitutional supercooling diagram: typical Nb distribution in a melt – a), schematic part of the phase diagram – b) and liquidus temperature distribution and thermal gradients in the melt – c)

During DED, the microstructure significantly influences the properties of the printed wall. The evolution of this microstructure is fundamentally tied to the solidification process. By examining the phase diagram for INCONEL 625 (referenced in Fig. 34), we can analyze constitutional supercooling, particularly for niobium (Nb), a key element in this alloy (Ref. 42, 43).

Constitutional supercooling is a well-understood mechanism in metallurgy. A general sketch of this phenomenon is depicted in Figure 35. The concept of constitutional supercooling, as laid out in seminal articles ((Ref. 27, 28)), fundamentally describes a condition where the actual temperature in the melt pool is less than the liquidus temperature near the solidification interface. This condition leads to instability in the planar solidification front.

In the context of INCONEL 625, segregation leads to the redistribution of Nb within the melt pool (as illustrated in Fig. 35 a). Combined with the negative slope of the liquidus line in the phase diagram (Fig. 35 b), this segregation results in instantaneous undercooling within the melt (Fig. 35 c). As a consequence of this undercooling, the initially flat solidification front becomes unstable, giving rise to nonhomogeneous perturbations that eventually form the observed nonhomogeneous structures.

This understanding of constitutional supercooling in the context of DED is critical for controlling the microstructure of INCONEL 625. By managing the distribution of elements like Nb and controlling the temperature conditions within the solidification zone, it's possible to influence the microstructure formation, thereby affecting the mechanical properties and overall quality of the printed material.

The value G/R (Fig. 33) may be considered as a bifurcation parameter. The solidification front is stable at the condition:

$$G/R > \Delta T/D_L, \quad (15)$$

where G is the temperature gradient (K/m) in the liquid, R is a solidification front velocity, ΔT is the equilibrium solidification temperature range, and D_L represents the solute diffusion in a melt. The value G/R as a solidification parameter determines the morphology of the microstructure (see the sketch plot in Fig. 33). One can see that for a large gradients no instability occurs. That is why as it follows from Kurz and Fisher the threshold for planar solidification is (Ref. 26, 44).

$$G/R = \Delta T/D_l = 7000K \cdot s/mm^2, \quad (16)$$

In the opposite limit the planar front becomes unstable and columnar and dendrite structures occur

$$G/R < \Delta T/D_L, \quad (17)$$

In the realm of DED and its impact on microstructure, the ratio of the thermal gradient (G) to solidification rate (R) plays a pivotal role. A smaller G/R ratio leads to greater undercooling and, consequently, smaller morphological patterns during solidification. Essentially, a higher solidification rate results in finer structures.

When the G/R ratio is sufficiently low, nucleation of the solid phase occurs throughout the melt volume, leading to the formation of equiaxed structures. This phenomenon contrasts with conditions where the G/R ratio is higher, favoring planar front solidification and resulting in different morphological outcomes.

Now, applying the insights from the previous section, we consider the thermal gradient G in the vicinity of the mushy zone. As illustrated in Figures 10 to 13, the lowest G is typically found near the upper surface of the melt pool, with the highest G at the bottom. The solidification velocity R is influenced by the laser scanning velocity v and the angle between the melt pool's normal and the laser's propagation direction.

We thus observe two limits of planar front solidification: one where the front remains stable at large gradients (as seen in Equation 16) and another where equiaxed grain growth prevails at lower thermal gradients and high R values. Between these two extremes lies a spectrum of possible melt pool grain structures.

4.3 The Columnar to Equiaxed Transition (CET)

An important aspect of DED microstructure is the Columnar to Equiaxed Transition (CET). We aim to estimate the CET by correlating solidification parameters with the evolving microstructure. This involves understanding the grain growth mechanisms during the solidification of the molten pool.

Our findings suggest that increasing the laser power and scanning speed facilitates the CET process, leading to the formation of equiaxed structures. This relationship between the operational parameters of DED (like laser power and scanning speed) and the resulting microstructure aligns with the mechanisms and observations reported in previous studies (Ref. 45–51). This understanding is important for tailoring the microstructure during DED processes, allowing for greater control over the mechanical properties and quality of the final printed material.

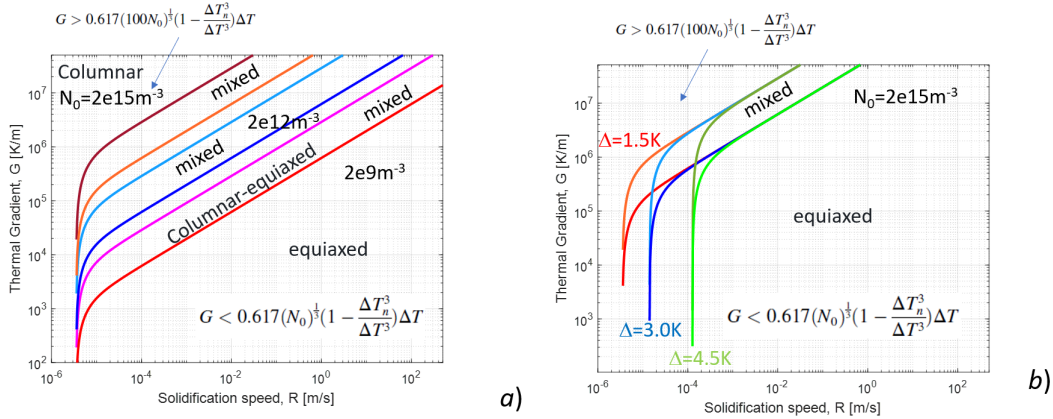


Figure 36.—The columnar to equiaxed transition diagram for INCONEL 625 parameters depending on initial nucleation concentration – a). The CET plot for different values of undercooling – b)

In the study of DED, the relationship between the primary dendrite tip growth velocity and the columnar microstructure is critical. This relationship can be understood through the work of Hunt, which provides equations to establish the conditions under which columnar growth is realized (Ref. 49, 50).

The criterion for constitutional supercooling for plane front instability, derived from Hunt's work, suggests that columnar growth occurs when the thermal gradient (G) is greater than a certain threshold. This threshold is defined by the equation:

$$G > 0.617 \times (100 \cdot N_0)^{1/3} \times \left[1 - \frac{\Delta T_n^3}{\Delta T^3} \right] \times \Delta T, \quad (18)$$

where N_0 is the nuclei density, ΔT_n is the instantaneous nucleation undercooling, and ΔT is the columnar structure front undercooling.

Constitutional dendrite tip undercooling, ΔT_c , for both columnar and equiaxed dendritic growth, can be approximated using Hunt's equation (Ref. 49, 50):

$$\Delta T = \Delta T_c = (a \times V)^{1/n}, \quad (19)$$

where V is the dendrite tip velocity, and a and n are constants that can be determined using

geometrical arguments proposed by Kurz et al.

Furthermore, Hunt's model also defines the critical gradient for fully equiaxed grain growth, G_c , which depends on nuclei density and undercooling:

$$G_c = \Delta T \times N_0^{1/3}. \quad (20)$$

In Hunt's original paper, the value of n was taken as 2. However, further analysis for high-velocity scenarios suggests that $n = 3.4$ and $a = 1.25 \times 10^6$ [K^{3.4}/ms] provides a more accurate representation. This leads to a final expression for solidification under high temperature gradients, which is essential for understanding DED processes (Ref. 51, 52):

$$\frac{G^n}{V} = a \times \left[\frac{-4\pi \times N_0}{3 \times \ln(1-f)} \right]^{n/3} \times \left(\frac{1}{1+n} \right)^n, \quad (21)$$

where f represents the fraction of equiaxed nuclear grains ahead of the advancing solidification front, influencing the formation of either columnar or equiaxed structures.

From the thermal gradient G , solidification velocity V , and cooling rate ϵ , it is possible to predict the microstructure type. This relationship is exemplified in Figure 37, which tracks the thermal gradient at different points within a sample, correlating with melt pool dynamics and detailed cooling rates as shown in Figures 38 and 39.

The analysis of these various parameters and their interplay provides insights into the formation of microstructural patterns in DED-manufactured materials. By mapping these conditions on a CET map (Figure 36), one can predict the likelihood of forming mixed or equiaxed structures at different locations within the solidification region, important for optimizing the DED process and achieving desired material properties.

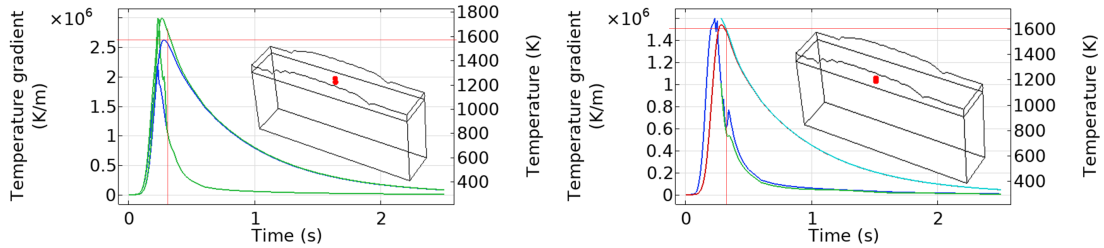


Figure 37.—Thermal gradient and Temperature evolution in two points close to the melt pool solidification boundary located at the wall center (left plot) and on the wall (right hand side, see two inserts to linear graph) showing that thermal gradient at the center is about two times larger than for side points.

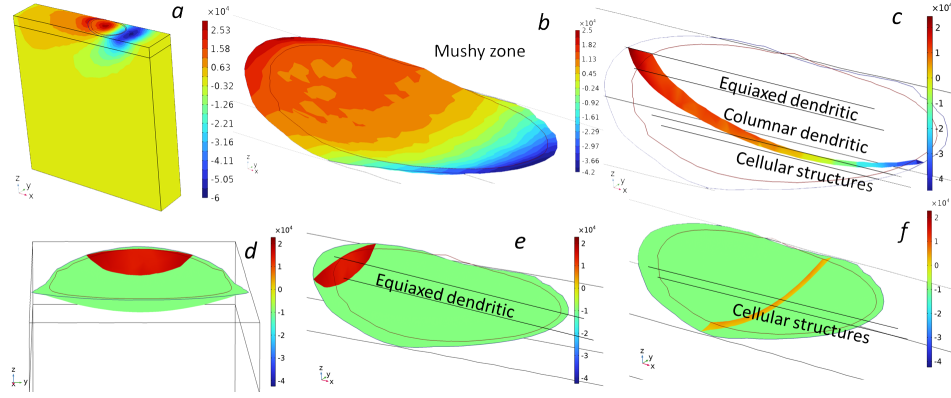


Figure 38.—Melt pool analysis: The cooling rate for the wall – a), Mushy zone cooling rate distribution – b), the microstructure localization along the melt pool cross-section, showing the possible evolution of the structures through the melt pool cladding domain – c, the substantial change in cooling rate (color changed from red to yellow) for the tail and bottom and side positions (red) – d), f) and e)

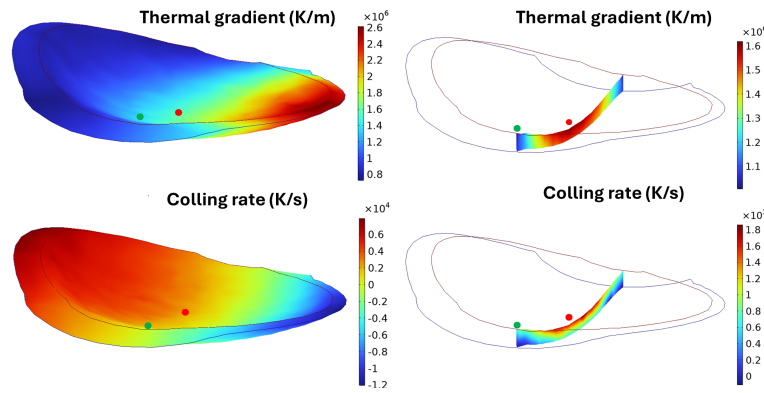


Figure 39.—Thermal gradient (first row) and cooling rate (second row) in the mushy zone. The points at the melt pool center and on a side are plots for convenience of the CET analysis

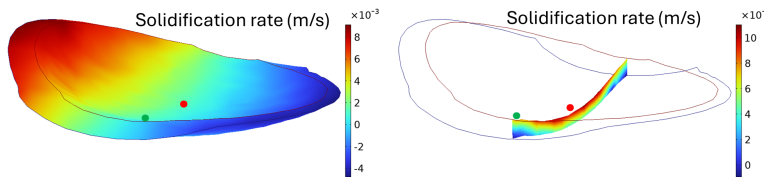


Figure 40.—Solidification velocity field in mushy zone – left, and cross-section of the zone for $V > 0$ and $G > 0$ – right

We are going to determine thermal gradients in the lateral direction across the thickness wall in different positions Fig. 41. Several lines are drawn along the laser beam propagation. The red line is close to the melt pool depth and the green one on the wall side surface is close to the top surface.

The results of the gradient distributions are presented on the right linear plot. The region of the nonlinearity is shaded by red color for the central melt pool depth and in green for the side green line. One can see the nonlinearity of the thermal gradient is localized at larger value (1.5×10^6 K/m) and for the plots for the side line (0.75×10^6 K/m). Certainly due to larger solid thermal conductivity gradient at the center is larger.

Since the sample is short we have a certain drift in location of these characteristic feature non-linear values. Similar computer experiment was done for a longer sample with the same processing parameters. The results are presented in Fig. 42 where three linear plots are presented along the three lines: blue, red and green. Starting from one third of the length the nonlinear N-shaped feature is practically constant. This feature characterises an almost stationary thermal gradient distribution. The final microstructure can be characterized by this. Localization of the N-shaped part is largest for the red line at the center and is the deepest melt pool formation at the center. The thermal gradient on the surface on the top of that line is smaller and comparable to the wall side gradient which is characterised by the largest nonlinear shape. As a result, thermal gradients near the free surface (top and side) are comparable from the standpoint of cooling since they are determined by the convective cooling surface. At the same time they are approximately two times smaller than the thermal gradient near the melt pool depth (red line, Fig. 42).

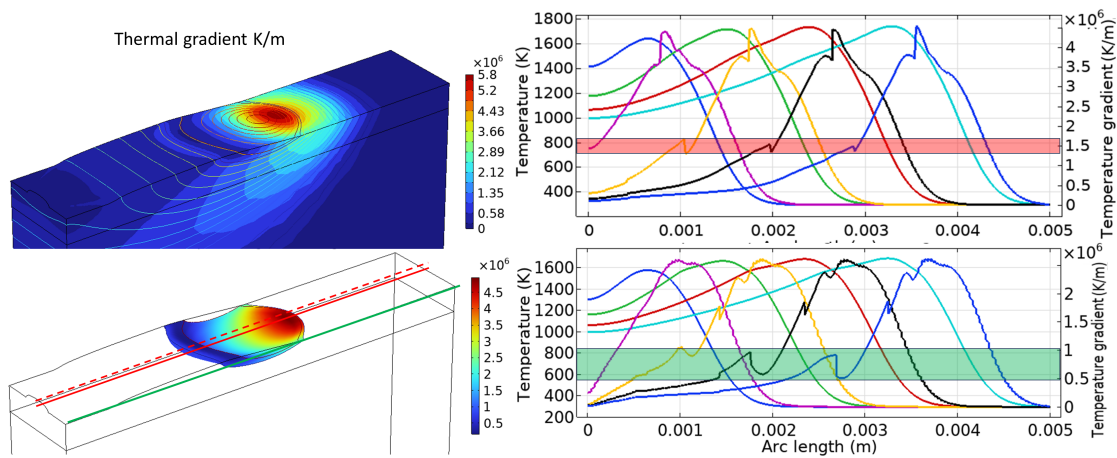


Figure 41.—Thin wall formation model for height $h=4$ mm. The temperature distribution at $t=0.425$ s – left-hand side plot, Temperature and thermal gradient distributions at times moments $t=0.05$ s, 0.15 s, 0.25 s, 0.35 s taken along the path in the middle of the top surface – middle line plots, and thermal gradients in the mushy zone.

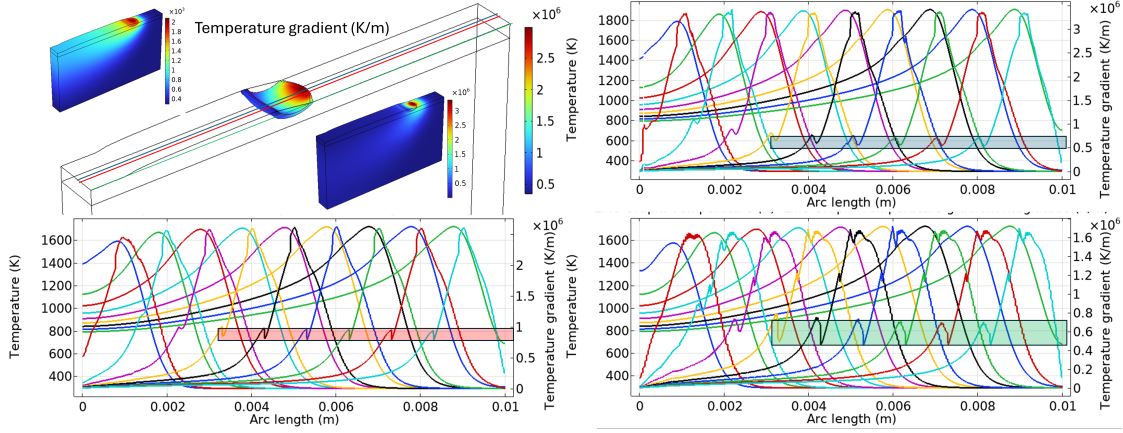


Figure 42.—Thin wall formation model for height $h=4$ mm. The temperature distribution at $t=0.425$ s – left-hand side plot, Temperature and thermal gradient distributions at times $t=0.10$ s, 0.20 s, 0.30 s, 0.40 s, 0.50 s, 0.60 s, 0.70 s, 0.80 s, 0.90 s taken along the path in the middle of the top surface – middle line plots, and thermal gradients in the mushy zone

The DED manufacturing process for INCONEL 625 was also simulated to analyze solidification cooling rates within the mushy zone, focused on variations across the solidification domain for a taller wall (Fig. 43, 44). In this simulation, a wall with geometric parameters (5 mm length, 1 mm thickness, and 5 mm height) was modeled, starting with an initial temperature of 293 K and consistent heat convection parameters.

Analyzing a thermal gradient, cooling rate and temperature along the line on the top wall surface, translated it deeper to capture melt pool depth and to the wall's top to assess vertical differences. Shifting the path to the wall's side, as shown in the plot, facilitated comparison of PDAS variations in the lateral direction. Subsequent analysis of results along these lines elucidated parameters essential for microstructure determination, forming a comprehensive map of thermo-physical parameters. A significant advantage of this method lies in its mathematical models ability to accommodate the free form of the cladding domain. This approach can be applied practically to any one-bead wall, demonstrating how parameters vary with factors such as cladding domain, wall height, and thickness.

In the first row, temperatures (dashed line), thermal gradient, and cooling rate along the path on the top surface are depicted. Notably, the thermal gradient at the solidus surface measures approximately $6e5$ K/m, with a cooling rate of nearly $4e3$ K/s. The second row presents a zoomed-in view of the same variables along the path, extending down (-100 μm) and $+250$ μm up from this line. Observations reveal that thermal gradients increase for melt pool depth, while cooling rates decrease. Conversely, at the top of the cladding domain, thermal gradient remains relatively stable compared to the top surface line, yet the cooling rate nearly doubles compared to the bottom line. The thermal gradients and cooling rates decrease a little (about 10%) by translation a path line to the side wall comparing to initial path at the center of the wall.

The analysis concludes that maximum gradients occur at the solidus surface of the mushy zone domain during cladding. Moving the path to the top surface of the cladding DED domain results in minimal gradient changes, while the cooling rate increases to almost $6e3$ K/s on the top surface. Mapping these findings to PDAS size suggests an average microstructure size of approximately

5 μm (ranging from 4.5-5.5 μm) throughout the melt pool cladding domain. Near the bottom melt pool surface, the microstructure size may be slightly larger, and for the top surface, it may be slightly finer. Although the developed technique enables precise PDAS prediction, averaging yields a reliable estimation of 5 μm , despite potential variations for the larger wall thicknesses not presented here.

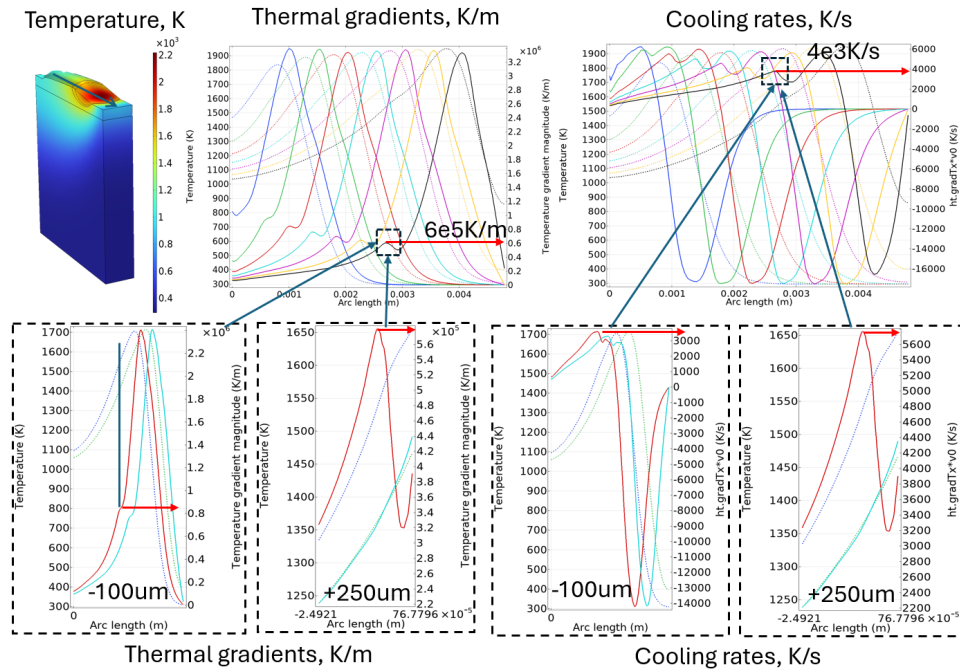


Figure 43.—In the first row from the left to the right one can see the simulation domain, the temperature and thermal gradient magnitude with the step $t=0.1$ s and last plot is a temperature and cooling rate for the same steps. The second row is devoted to zoomed region in the solidus surface for the path shifted from its initial position 100 μm down and 250 μm up reflecting molted cladding domain.

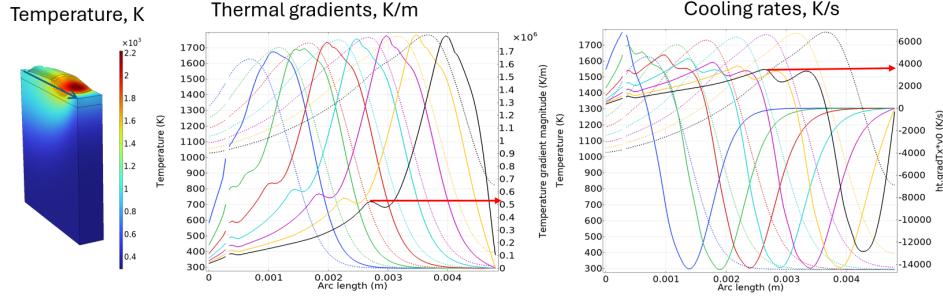


Figure 44.—From the left to the right: the simulation domain, the temperature and thermal gradient magnitude with time step $t=0.1$ s and the last plot is temperature and cooling rate for the same steps. These data are the result of the solidus surface for the path shifted (first plot) to the side surface.

5 Liquid-Based DED Model Incorporating fluid flow and Marangoni Surface Tension Effect

In a previous section, the fluid motion was not taken into account in the melt pool, considering the properties of the solid and liquid to be similar differing by thermo-physical parameters. At the same time, the dynamics of the melt pool in DED is important for understanding and optimizing the process. To model these dynamics, the melt fluid flow was considered by solving Navier-Stokes equations. This approach allows calculation of the melt pool shape and understanding of the laminar flow within it, characterized by fluid velocity u and pressure p .

The Navier-Stokes equations for this scenario are expressed as follows (Ref. 9, 53–59):

$$\rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u = \nabla \cdot \left[-pI + \mu(\nabla u + (\nabla u)^T) - \left(\frac{2\mu}{3} - \kappa \right) (\nabla \cdot u)I \right] + F, \quad (22)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \quad (23)$$

where t is time, u_i is the i -th component of the velocity u , μ is the viscosity, p is the pressure, T is the temperature, ρ is the density, and κ is the thermal conductivity.

The volumetric force term F arises from (Ref. 57, 58):

$$F = \frac{(1 - f_l)^2}{f_l^3 + \varepsilon} A_{mush}(u - u_0), \quad (24)$$

where f_l represents the volume fraction of the liquid phase,

$$f_l = \begin{cases} 0 & \text{if } T \leq T_s, \\ T - T_s & \text{if } T_s < T < T_l, \\ 1 & \text{if } T_l \leq T. \end{cases}$$

where A_{mush} and ε are constants, with A_{mush} being large and ε small ($\sim 10^{-3}$). These constants effectively freeze the motion of the metal while it is in the solid phase. This justifies a rigid assumption for a solid phase where the material has a zero velocity in the solid zone. The parameter

f_l is zero in the solid and a unit value in the melt. In the denominator, $A_{mush} = 10^6$ have been adopted in order to avoid divergence. The volume force vector F related to buoyancy and gravity is given by:

$$F = g\rho_0(1 - \beta(T - T_0)), \quad (25)$$

where ρ_0 is the density, g is gravity at the reference temperature, and β is the thermal expansion coefficient.

The surface of the melt in an atmosphere should take into account the surface tension. In this case the temperature difference along the free boundary leads to the gradient of the surface tension. As a result, the tangential force driven by the surface tension gradient must compensate the viscous force of the flow due to shear. The stress tensor is defined in terms of the local fluid pressure and velocity field (Ref. 5):

$$\mu \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial \sigma}{\partial \boldsymbol{\phi}} = \frac{d\sigma}{dT} \frac{\partial T}{\partial \boldsymbol{\phi}}, \quad (26)$$

where $\mathbf{n}$ and $\boldsymbol{\phi}$ denote the unit outward normal and tangential vectors to the free surface. The hydrodynamic stress at the surface must balance the tangential stress associated with gradients in σ . Marangoni flows, caused by surface tension gradients, play a significant role in the DED process. Surface tension σ depends on the temperature and chemical composition at the interface. In this study, Marangoni flows are generated by temperature gradients. The tangential stress balance at a free surface is described by (26) which can be rewritten in:

$$\mu \frac{\partial u}{\partial n} = \frac{\partial \sigma}{\partial T} (\nabla T - \mathbf{n}(\mathbf{n} \cdot \nabla T)), \quad (27)$$

The hydrodynamic stress at the surface must balance the tangential stress associated with gradients in σ .

This comprehensive approach, integrating the Navier-Stokes equations with considerations for Marangoni flows, provides a detailed model for analyzing the fluid dynamics within the melt pool of DED processes. Understanding these dynamics is essential for controlling the microstructure and mechanical properties of the printed material.

The heat balance part is practically the same as considered by equations (1)–(5).

5.1 Simulation results

The simulation approach presented in this section is similar to previous. The only difference was that moving mesh in COMSOL was used instead of the deformable domain. Different simulation results are presented in Fig. 46–51, which will be described later.

In Fig. 45 the initial mesh as well mesh deformation is presented on the left and a corresponding velocity solution on the right. The velocity reaches $5 \cdot 10^{-2} m/s$ in the melt pool. It is pretty obvious that this approach has little difference from the liquid based approach that does not resolve boundary layer shear flows which require a much finer mesh.

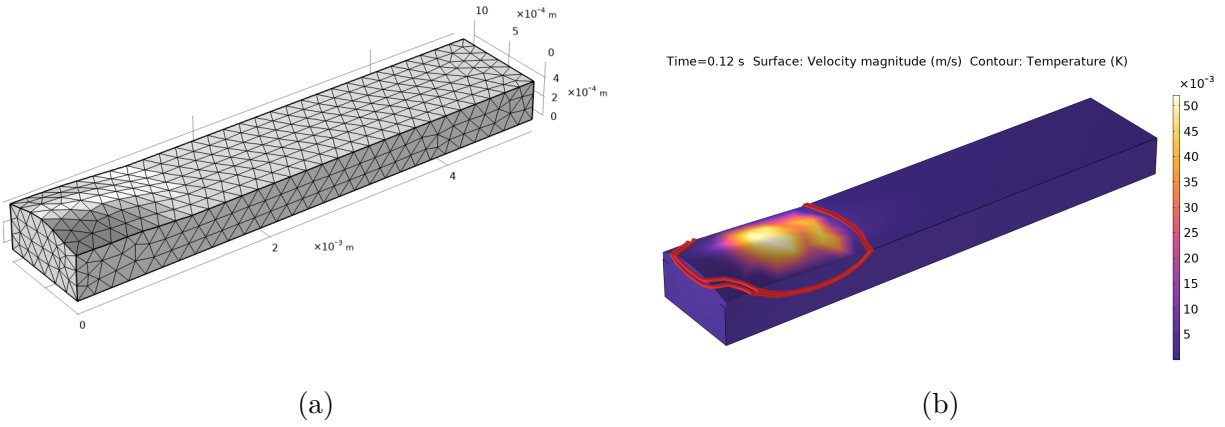


Figure 45.—The first layer formation: deformable mesh – a), and magnitude of the velocity – b)

The temperature and velocity magnitude distribution for a certain time frame ($t=0.35$ s) are presented in Fig. 46 and 47.

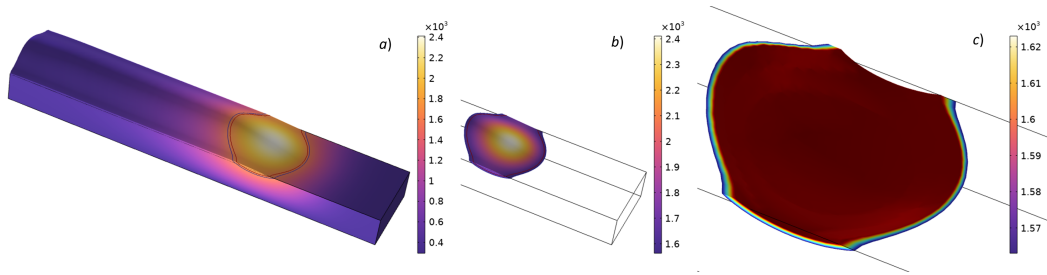


Figure 46.—Thin wall formation model: The temperature of the domain at $t=0.35$ s – a), Melt pool domain in a sample – b and zoomed mushy zone – c

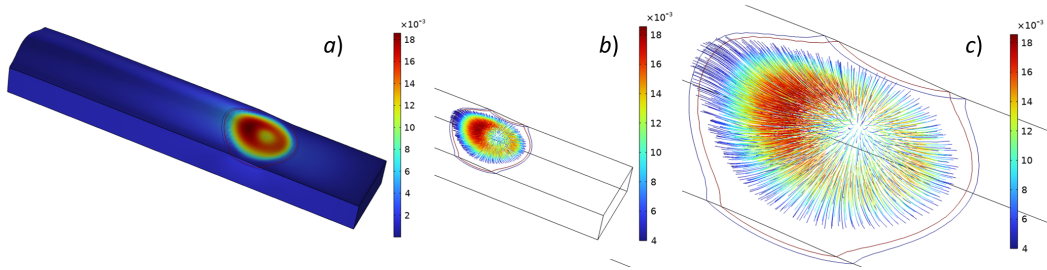


Figure 47.—The velocity magnitude showing that it is zero in all domain (frozen state) except in the melt pool where the velocity is substantial – a), vector plot for velocity gradients – b and – c)

The next three plots show how the deposition velocity changes the shape of the cladding domains

increasing the heights of them with increasing the deposition rate.

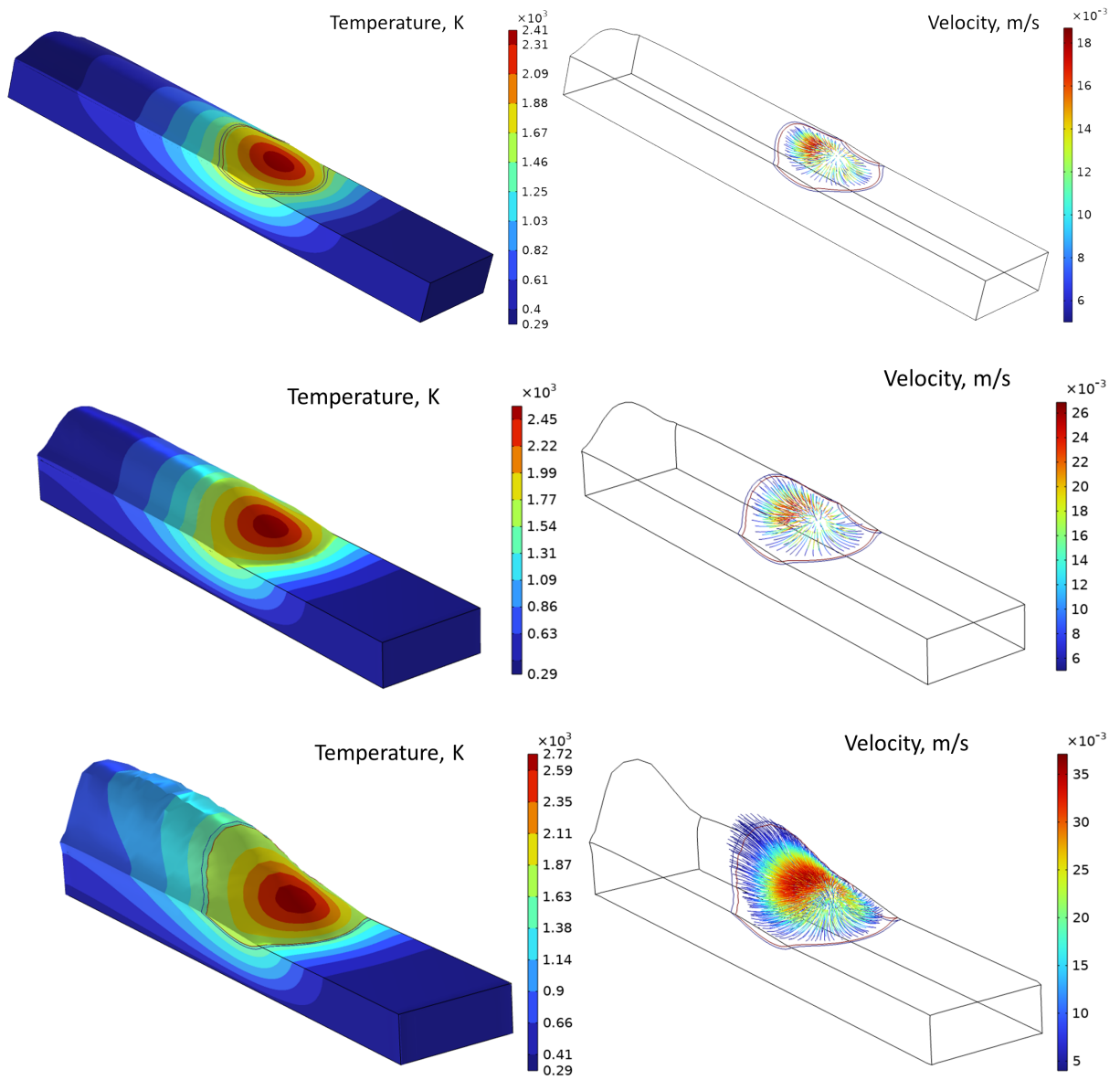


Figure 48.—The first layer temperature formation: the temperature is presented in the first column and velocity vector components in the second one. The deposited velocity for the first row is 1 mm/s, the second one is 2 mm/s and the last one is for the 3 mm/s

To better understand velocity distribution in the cladding melt pool domain the longitudinal cross-section is shown in Fig. 49

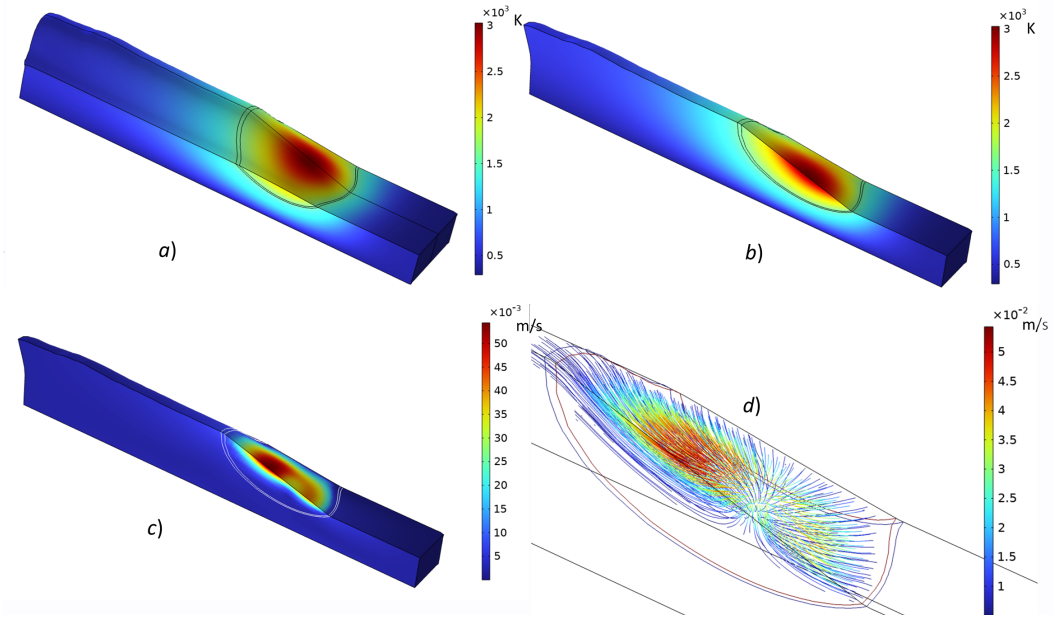


Figure 49.—Temperature distribution at $t=0.35$ s – a), The cross-section of the temperature – b), cross-section for velocity magnitude – c) and zoomed melt pool velocity stream lines – d)

As an example of multilayered cladding formation is presented in Fig. 50 and 51. In Figure 50 the mesh before deposition is presented (left plot) and the mesh distribution for after 10 layers (right hand side). In Fig. 51 some successive layer formation is presented.

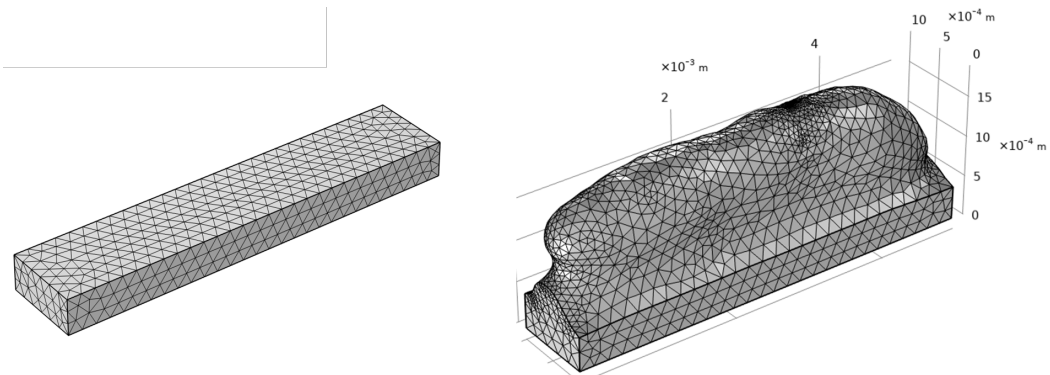


Figure 50.—Thin wall formation model: The initial mesh distribution – a) and the generated mesh for a 10-layer formation – b) for liquid based model

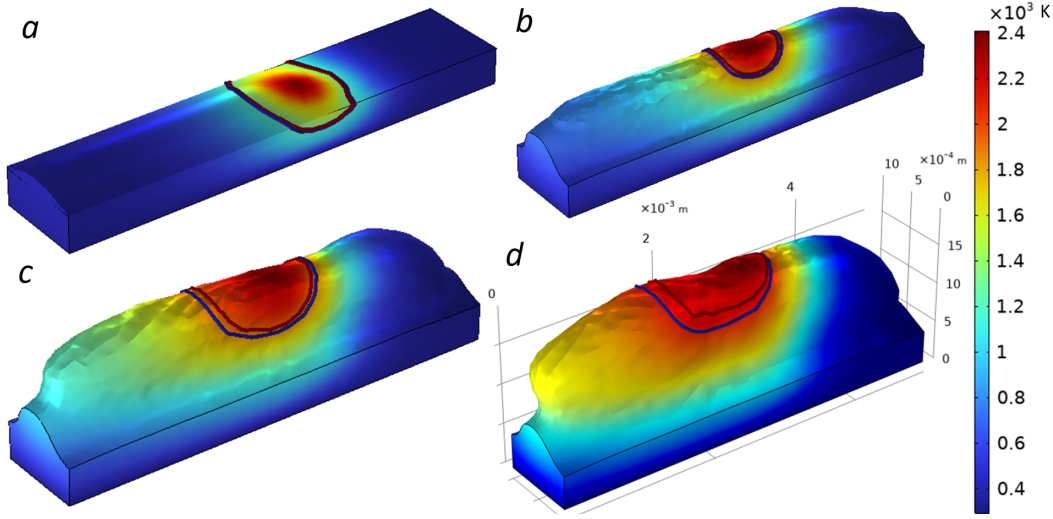


Figure 51.—Temperature distribution for different layers at $t=0.3$ s: the first layer – a), 6-th one – b), 10-th – c) the 14-layer – d). The 14 layer is displayed with indication geometrical parameters of the wall.

Since the simulation approach for the liquid-based model is not significantly different from the previous consideration, all the conclusions drawn before are equally applicable to this one.

6 Residual Stresses

Simulating residual stresses in DED processes involves computationally modeling structural mechanics to predict the deformation and stress evolution within the material. This procedure relies on transient thermal analyses conducted in previous sections, which accounts for the temperature history of the material during deposition and subsequent cooling. This considers factors such as laser heat input from the energy source and heat dissipation to the surroundings.

Mechanical analysis is then performed by incorporating thermal expansion, phase transformation, and material plasticity effects. This involves solving the equations governing the mechanical behavior of the material under the applied thermal loads. Residual stresses arise from thermal gradients, phase transformations, and plastic deformation accumulated during the DED process. While the developed DED modeling approach isn't extensively tailored for simulating residual stresses in multilayered structures, this section discusses its key features.

In the context of DED processes, understanding and controlling the formation of residual stresses is important for predicting these stresses in actual structures. These stresses emerge from thermal expansion and contraction as materials undergo heating and cooling during the printing process. Accurately predicting residual stresses in manufactured parts requires considering the plastic component.

The momentum balance equation governs the stress deformation problem, especially under quasi-static conditions (Ref. 1, 3, 4, 9)

$$\nabla \sigma(u) + f = 0, \quad (28)$$

where $\sigma(u)$ is the second order elasticity tensor stress depending on the displacement field u , and f represents body forces.

The mechanical constitutive law for elasticity is described by:

$$\sigma = C : \epsilon, \quad (29)$$

where C is the fourth order material stiffness tensor, and σ and ϵ are the second order stress and elastic strain tensor, correspondingly. The total strain experienced by the material during the DED process is a combination of plastic strain ϵ_{pl} , elastic strain $\epsilon = \epsilon_{el}$, and thermal strain ϵ_{th} :

$$\epsilon_{tot} = \epsilon_{el} + \epsilon_{pl} + \epsilon_{th}. \quad (30)$$

Thermal stress changes during deposition are governed by:

$$\sigma_{th} = \alpha \Delta T \cdot I, \quad (31)$$

where σ is the stress in the heated domain following temperature variations, and α is the coefficient of thermal expansion (CTE), which is a function of the temperature, ΔT is a temperature difference, and I is the identity matrix.

6.1 Simulation results for single bead layer

Residual stresses are a characteristic result of the AM process. These stresses can lead to plastic deformation if they exceed the material's yield stress or cause plastic flow if they surpass the local ultimate tensile strength. In DED, tensile residual stresses are often significant along the laser scanning direction, especially in the top layers, potentially affecting the strength properties of these layers. Understanding how these stresses vary with deposition thickness is an important area of study.

Our model examines the tensile stress in the direction of the laser scanning depending on the deposition thickness. Optimal residual stress properties are likely achieved with the minimum cooling rate during solidification.

The formation of residual stress for two different layer thicknesses is depicted in Figure 52. These differ in cladding melt velocities: the first structure (a) has a thinner layer, while the second (b) is thicker. Despite these differences, the residual stresses after printing appear similar. This similarity is attributed to the comparable thermal histories experienced during the manufacturing of these layers, leading to analogous final residual stresses.

Understanding and predicting residual stresses are essential for ensuring structural integrity and mechanical performance of parts produced using DED. Simulations may provide valuable insights for process optimization.

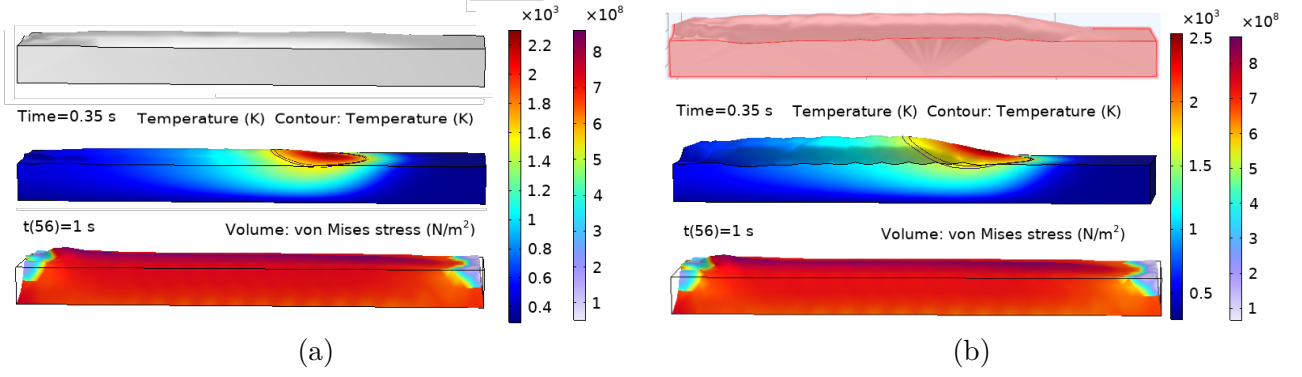


Figure 52.—Melt pool plots for two different layer thicknesses: $v_d = 1 \text{ mm/s}$ – a), and $v_d = 2 \text{ mm/s}$ – b). $Q = 1.75 \cdot 10^8 \text{ W/m}^2$, all other parameters are the same

The residual stress formation for walls of different heights are presented in Fig. 53, 54, 55. First row shows the temperature at time 0.4 s and at the final time when the layer has cooled down. The residual stress for this terminal time is presented in the second row. The stress Sxx (plot c) is localized close to the top surface while von Mises stress (plot d) shows that all components of the stress arise and lead to deformation of the wall.

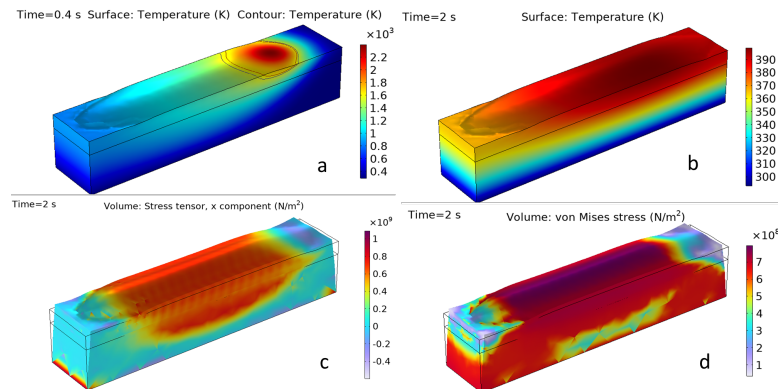


Figure 53.—Temperature distribution for $t=0.4 \text{ s}$ – a) and terminal time $t=1.5 \text{ s}$ – b, residual stress Sxx – c) and von Mises stress – d) after cool down stage (fig. b)

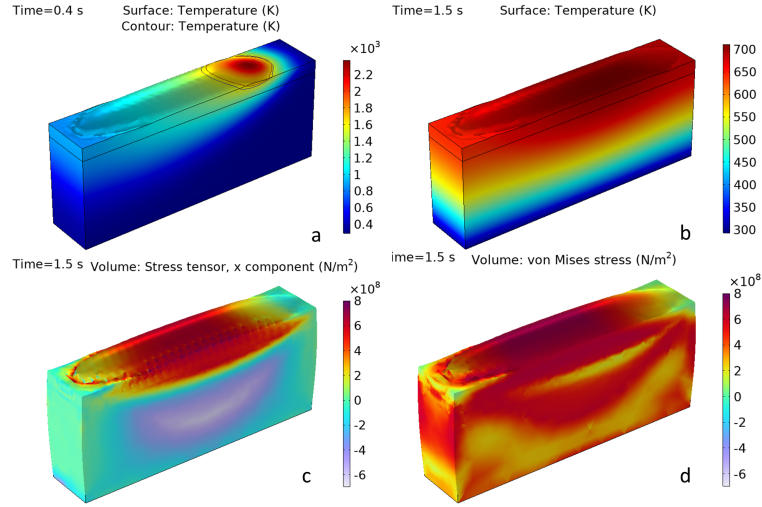


Figure 54.—Temperature distribution for $t=0.4$ s – a) and terminal time $t=2.0$ s – b, residual stress S_{xx} – c) and von Mises stress – d) after cool down stage (fig. b).

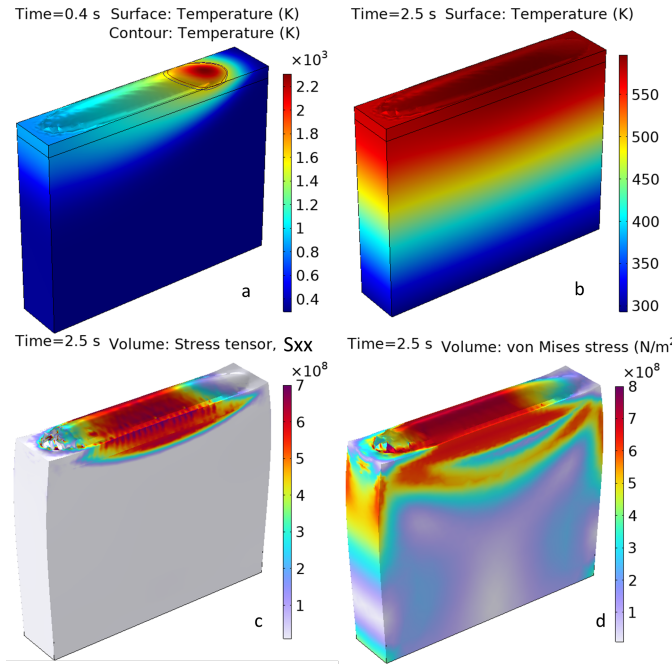


Figure 55.—Temperature distribution for $t=0.4$ s – a) and terminal time $t=2.5$ s – b, residual stress S_{xx} – c) and von Mises stress – d) are presented after terminal time.

Our studies have shown that factors such as wall height and inter-layer dwell time significantly impact the residual stress in fabricated structures. For instance, increasing the dwell time, which allows the wall to thermally equilibrate with room temperature, results in a notable increase in residual stress, from 400 MPa to 750 MPa. This finding is highlighted in the results shown in Figures 53 to 55.

Tensile residual stresses, particularly in the last few layers of a DED manufactured wall, tend to be significant along the laser scanning direction. These high stress levels can potentially weaken the strength properties of these layers. Our model aims to explore the relationship between tensile stress and deposition height. It appears that optimal residual stress properties are likely to be achieved with a minimal cooling rate during the solidification process.

6.2 Residual stress results for single bead wall during successive cladding

Figures 56 to 58 present simulation results for successive layers. These simulations consider the residual stress from one layer as a pre-stressed state for the next layer's modeling. This approach allows for a more comprehensive understanding of how residual stresses accumulate and interact across layers in a DED process.

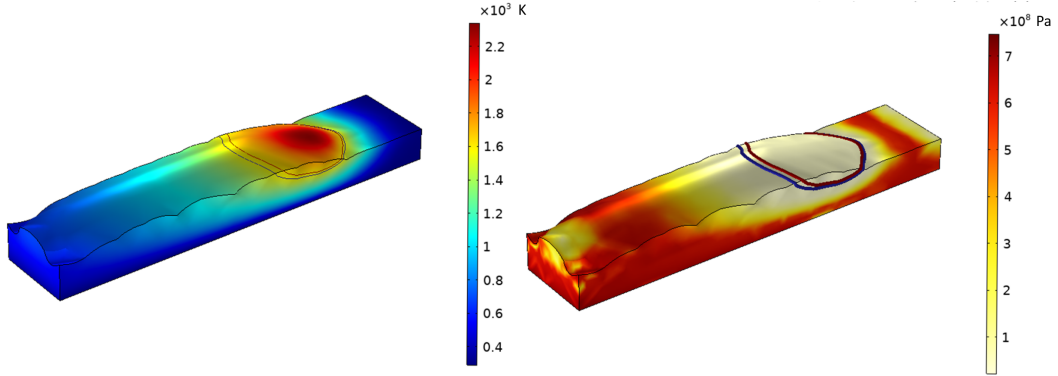


Figure 56.—Temperature distribution – a) and von Mises stress – b) for solid shaped model after 1st layer manufacturing. Snapshots are taken at the time $t=0.4$ s, melt pool domain is single out by solidus and liquidus lines

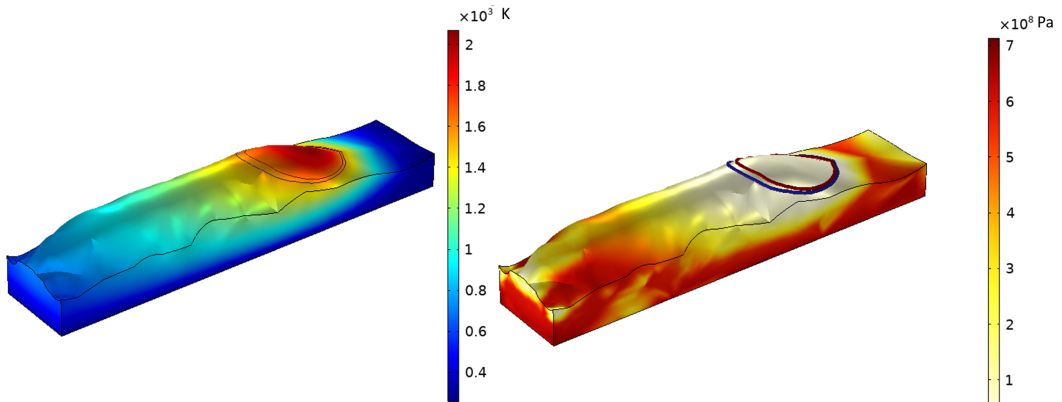


Figure 57.—Temperature distribution – a) and residual stresses – b) for the second layer manufacturing. Snapshots are taken at the time $t=0.4$ s, melt pool domain is single out by solidus and liquidus lines

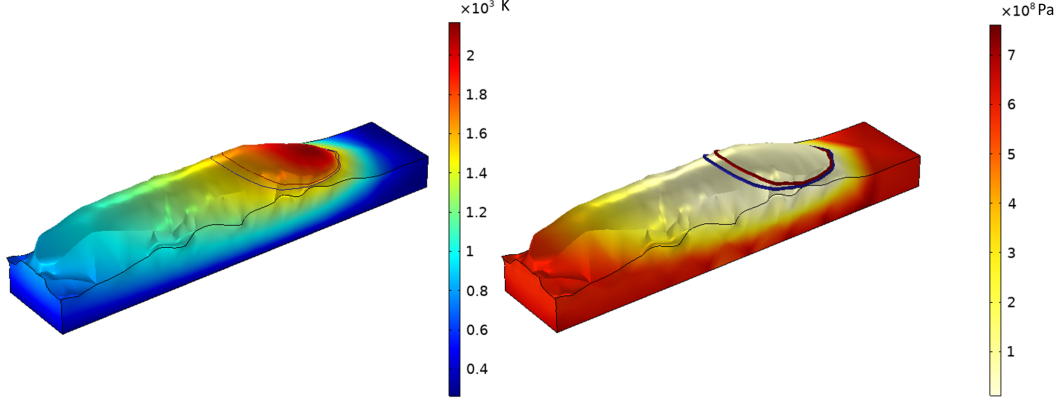


Figure 58.—Temperature distribution – a) and residual stresses – b) for the third layer manufacturing. Snapshots are taken at the time $t=0.4$ s, melt pool domain is single out by solidus and liquidus lines

The insights gained from these studies are pivotal for improving DED process parameters. By carefully managing factors like dwell time and understanding the implications of successive layers, manufacturers can better control the residual stresses in their products, leading to improved mechanical properties and reliability.

7 Deposition at an angle to the surfaces for single bead wall track

The models initially developed for vertical powder deposition have been adapted to determine the shape of the cladding material at various angles. This updated model enables studying the evolution of the surface shape of DED cladding when external forces are applied. For instance, consider the cladding shape and melt pool formation when the sidewalls are not parallel to gravity. The two-layer cladding is presented in Figure 59 for a 45-degree surface slope. It is evident that gravity-driven melt flow begins to generate nonsymmetric shapes right from the start of the laser scan.

The modeling of the clad shape evolution is performed using two types of models: solid-based (Figure 60) and liquid-based (Figure 61) which are presented in a front view as the clad domain moves towards the viewer. A 45-degree angle was used to demonstrate that our developed model is capable of predicting surface evolution, a capability that other models, such as those with domain activation, may not possess.

We consider no powder loss during the sloped catchment of the powder but rather depend on the gravity-driven melt (solid) deformation of the deposition geometry. As it is shown, the wall's free-form deposited track is deformed, resulting in a specific deposition geometry (Fig. 60 – 61).

The developed fluid dynamics model is used to simulate the shape of the free form and melt pool, which can be useful for predicting the final deposition geometry in the DED process (Figure 61). In DED settings, this consideration might not apply to flat surfaces where the gravity force is orthogonal to the surface. However, cladding depositions might be necessary for sloped surfaces where gravity forms an overhang angle with the building surface. Here, the shape geometry is studied to predict the final deposition geometry, which will certainly be a function of the deposition angle. As a result, we obtained loss of symmetry in the cladding material during the DED process.

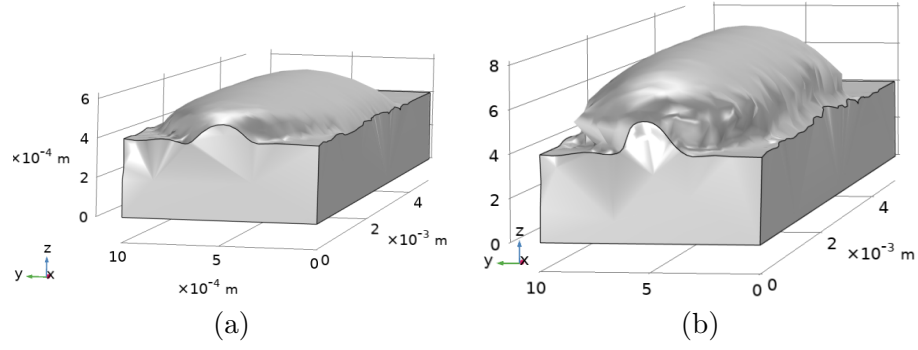


Figure 59.—The comparison of the free surface shapes for the gravity in normal direction – a), and gravity directed at 45 degree – b)

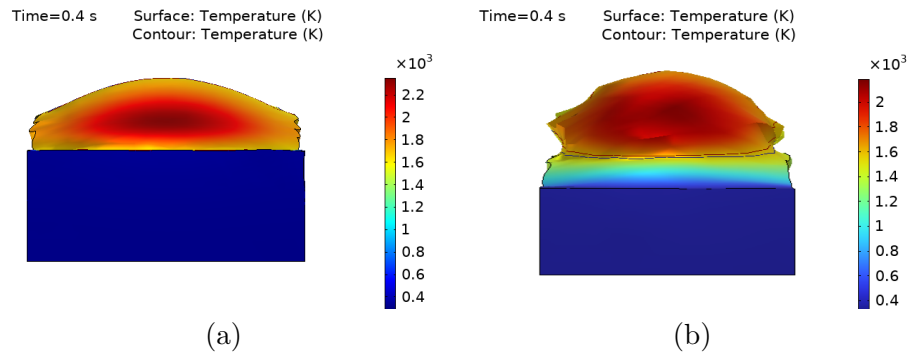


Figure 60.—Front view of the clad domains for solid based model: 1st layer – a), and 2nd layer – b)

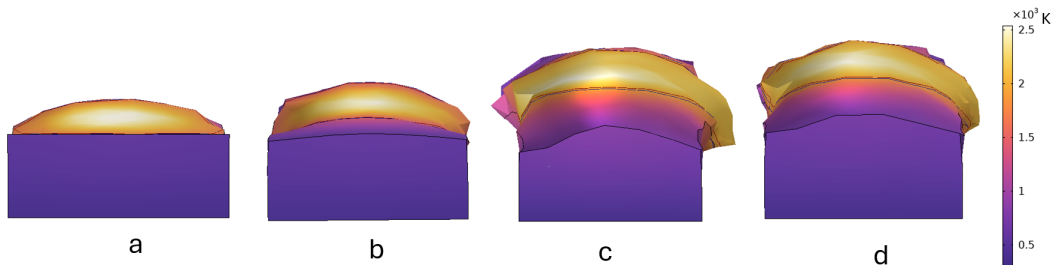


Figure 61.—Deformation of the DED layers during inclined gravity with overhang angle 45 Degree: first layer – a), second layer – b), third layer – c), fourth layer – d).

One can observe, particularly from Fig. 61, that each successive layer is inclined relative to the previous one. As more layers are added with inclined gravity, increasingly sloped overhang

geometry is produced.

No specific study has been conducted on modeling DED with inclined geometry. The aim was to demonstrate the capability of the developed multilayered model to account for layer manufacturing when laser melted powder deposition is not aligned with gravity, potentially leading to the formation of overhang structures. The conventional approach implemented in specialized commercial software such as Ansys Additive and Abaqus (3dExperience) do not reflect this issue. This study could be significant for repairing manufactured structures by adding additional layers inclined to the existing ones.

8 Discussion

This report proposes a new modeling approach for layer generation in AM manufacturing. A distinctive feature is that the build shape and mesh are not pre-existing but are deformed during simulation to model material addition. The modeling findings demonstrate the trackability of melt pool solidification parameters during the AM process. In this context, microstructure parameters, especially PDAS, can be predicted. The model effectively predicts microstructure parameters through thermal gradient (G), cooling rate (ϵ), and solidification front velocity (R). The interplay between these parameters facilitates the generation of a thermal process map, which is important for estimating the types and sizes of microstructure produced by the DED process.

The report illustrates how this approach can be used for studying cooling rates and thermal gradients during layer formation in multilayered structures. While the main advantage lies in developing a framework applicable to any DED simulation, the presented examples show the expected results from using this approach. The modeling process not only extends our understanding of the physics and characteristic parameters but also advances our understanding of material properties and printing techniques. The simulation findings complement other research and shed light on important details previously overlooked.

However, the layer-by-layer simulation approach may have limitations for modeling multilayer wall structures. Projection of results, such as final temperature or stress, from one domain to the next can be slow and decrease modeling capability. This approach is suitable when variable parameters like temperature and stress history are not critical. For instance, while thermal simulations alongside deformable domain models are efficient and versatile, the COMSOL approach may become impractical if consideration of residual stress from layer to layer for multiple layers is required. Nevertheless, if time history during multilayered modeling is unnecessary, the simulation is notably fast.

The practical implications of this method are wide-ranging for any DED study requiring knowledge of melt pool parameters, cooling rates, thermal gradients, and microstructures. These insights might be important for DED manufacturing of new walls or repair procedures.

The primary focus here is on thin walls, approximately 1 mm thick. However, these results can be extrapolated to single bead structures by adjusting modeling parameters. Having an explicit and physically clear model enables recommendations on microstructure formation, print parameter optimization, material selection, and specific application model design. A clear understanding of the theoretical background of the modeling approach contributes to the theoretical understanding of 3D printing processes. Utilizing the new concepts for detailed melt pool dynamics expands existing knowledge of DED simulation approaches. Undoubtedly, due to its simplicity and speed, this model could be used for digital twin modeling directly or through reduced-order approximation. The ease

of changing material nonlinear parameters suggests that this model might be flexible for many AM modeling approaches, including PBF, which is not considered here.

9 Conclusion

This study provides as an example simulation of DED additive manufacturing processes, particularly focusing on modeling fabrication a single bead wall using INCONEL 625. Key conclusions and specific outcomes include the successful development of COMSOL Multiphysics models for DED simulation, incorporating various features to simulate mass and heat addition during DED processes. Solid and liquid-based models were utilized to derive the main parameters of the built wall, conducting simulations in a 3D domain under different process parameters.

Nonlinear dependencies of the thermo-mechanical material characteristics of INCONEL 625 were accounted for, leading to a more accurate and realistic simulation of the DED process. Numerous computational tests were conducted to model features arising during the DED process, showcasing the model's flexibility concerning wall thickness, layer height, scanning, deposition speeds, and other process parameters.

Our approach highlights the importance of modeling the free surface of the DED manufacturing process, providing a more accurate reflection of real manufacturing scenarios compared to the widely used generation activation approach. This report demonstrates that the implemented COMSOL Multiphysics DED model is convenient and effective for modeling DED manufacturing, thermal history, cooling rates, and residual stress for different cladding layer heights and other process parameters, making it a valuable approach to modeling DED processes.

References

1. I. Gibson, D. Rosen, B. Stucker, M. Khorasani. Additive Manufacturing Technologies. Third Edition. Springer Nature Switzerland AG, 2021.
2. E. Toyserkani, A. Khajepour, S. Corbin. Laser Cladding. CRC PRESS. 2005
3. Laser Cladding of Metals. edited by Pasquale Cavaliere. Springer. 2021.
4. Dong-Gyu Ahn. Directed Energy Deposition (DED) Process: State of the Art. International Journal of Precision Engineering and Manufacturing-Green Technology (2021) 8:703–742.
5. H.L. Wei et al. Mechanistic models for additive manufacturing of metallic components. Progress in Materials Science 116 (2021) 100703.
6. D. Svetlizky et al. Directed energy deposition (DED) additive manufacturing: Physical characteristics, defects, challenges and applications Materials Today Research. Volume 49, October 2021, Pages 271-295.
7. Y.L. Hu et al. Effect of solution heat treatment on the microstructure and mechanical properties of Inconel 625 superalloy fabricated by laser solid forming. Journal of Alloys and Compounds 767 (2018) 330-344.

8. M. J. Kim, Ch. Saldana. Thin wall deposition of IN625 using directed energy deposition. 48th SME North American Manufacturing Research Conference, NAMRC 48, Ohio, USA. Procedia Manufacturing 00 (2019) 000–000.
9. COMSOL Inc. (2024). COMSOL Multiphysics [Computer software]. Version 6.0. Available from: <https://www.COMSOL.com/>
10. V. Luzin, N. Hoyer. Stress in Thin Wall Structures Made by Layer Additive Manufacturing. Residual Stresses 2016 (2016).
11. N. Ali et al. Fabrication of Thin Walls with and without Close Loop Control as a Function of Scan Strategy Via Direct Energy Deposition. Lasers in Manufacturing and Materials Processing (2022) 9:81–101.
12. V. Nain et al. Development of an Elongated Ellipsoid Heat Source Model to Reduce Computation Time for Directed Energy Deposition Process. Front. Mater. 8:747389.
13. A. Kantaros et al. 3D Printing and Implementation of Digital Twins: Current Trends and Limitations. Appl. Syst. Innov. 2022, 5, 7.
14. ANSYS Inc. (2024). ANSYS Additive [Computer software]. Version 2024 R1. Available from: <https://www.ansys.com/products/additive>
15. Dassault Systèmes. (2024). 3DEXPERIENCE Platform [Computer software]. Version R2024x. Available from: <https://www.3ds.com/make/service/3d-printing-service>
16. Simufact Engineering. (2024). Simufact [Computer software]. Version 2024.1. Simufact Engineering. Available from: <https://www.simufact.com/simufact-additive.html>
17. V. Nain. Efficient thermomechanical modeling of large parts fabricated by Directed Energy Deposition Additive Manufacturing processes. <https://theses.hal.science/tel-03962675>.
18. P. Promoppatum et al. A Comprehensive Comparison of the Analytical and Numerical Prediction of the Thermal History and Solidification Microstructure of INCONEL 718 Products Made by Laser Powder-Bed Fusion. Engineering 3 (2017) 685–694.
19. F. Lia et al. Thermal and microstructural analysis of laser-based directed energy deposition for Ti-6Al-4V and INCONEL 625 deposits. Materials Science and Engineering A 717 (2018) 1–10
20. D. Rosenthal. The Theory of Moving Sources of Heat and Its Application to Metal Treatments, Transactions of ASME, vol. 68, pp. 849–866, 1946.
21. Yu Kong, Haihong Huang. Effect of intrinsic heat treatment on microstructure and hardness of additively manufactured INCONEL 625 alloy by directed energy deposition Materials and Design 224 (2022) 111279.
22. X.X. Yao, X. Gao, Z. Zhang. Three-dimensional microstructure evolution of Ti6Al4V during multi-layer printing: a phasefield simulation. journal of Materials Research and Technology 2022 ; 20 : 934–949.

23. Z. Liu, H. Qi. Effects of processing parameters on crystal growth and microstructure formation in laser powder deposition of single-crystal superalloy, *Journal of Materials Processing Technology* (2014).
24. F. Brueckner et al. Process characteristics in high-precision laser metal deposition using wire and powder. *J. Laser Appl.* 29, 022301 (2017)
25. L. Chechik, I. Todd. INCONEL 718 two ways: Powder bed fusion vs. directed energy deposition. *Additive Manufacturing Letters* 6 (2023) 100145.
26. W. Kurz, David Fisher. *Fundamentals of Solidification*. Trans Tech Publications Limited, 1998
27. W.W. Mullins, R.F. Sekerka. Morphological stability of a particle growing by diffusion or heat flow. *Journal of Applied Physics*. 1963;34(2):323-9.
28. W.W. Mullins, R.F. Sekerka. Stability of a planar interface during solidification of a dilute binary alloy. *Journal of Applied Physics*. 1964;35(2):444-51.
29. J. Strickland et al. On Directional Dendritic Growth and Primary Spacing—A Review. *Crystals* 2020, 10, 627.
30. H.S. Whitesell et al. Influence of solidification variables on the dendrite arm spacings of Ni-based superalloys *Metall. Mater. Trans. B*, 2000, vol. 31B, pp. 546–51.
31. A. S. Sabau and al, Fluid Dynamics Effects on Microstructure Prediction in Single-Laser Tracks for Additive Manufacturing of IN625. *Metallurgical And Materials Transactions B Volume 51b*, June 2020—1263
32. W. Kurz et al. Columnar to equiaxed transition in solidification processing, *Science and Technology of Advanced Materials* 2(1) (2001) 185-191.
33. W. Kurz and D. J. Fisher. Dendrite growth at the limit of stability: tip radius and spacing *Acta Metall.* 29, (1981) 11–20.
34. Y. Chen et al. Dendritic microstructure and hot cracking of laser additive manufactured Inconel 718 under improved base cooling. *J. Alloys Compd.* 2016, 670, 312–321.
35. N. Menon et al. A Comparison of Microstructure and Microhardness Properties of IN718 Fabricated via Powder- and Wire-Fed Laser-Directed Energy Deposition. *Materials* 2023, 16, 1129.
36. D.D. Erick Schlienger et al. Near Net Shape Production of Metal Components Using LENS, 1998.
37. A. Alhuzaima et al. Controlling microstructural and mechanical properties of direct laser deposited Inconel 718 via laser power. *Journal of Alloys and Compounds* 872 (2021) 159588.
38. P. Mohammadpour and A. B. Phillion. Solidification microstructure selection maps for laser powder bed fusion of multicomponent alloys. *IOP Conf. Series: Materials Science and Engineering* 861 (2020) 012005.

39. Y. Gao, M. Zhou. Superior Mechanical Behavior and Fretting Wear Resistance of 3D-Printed INCONEL 625 Superalloy. *Applied Sciences* 2018, 8.
40. T. Mukherjee et al. Dimensionless numbers in additive manufacturing *Journal of Applied Physics* 121, 064904 (2017).
41. R. W. Kozar et al. Strengthening Mechanisms in Polycrystalline Multimodal Nickel-Base Superalloys. *Metallurgical and Materials Transactions A* 40.7(2009):1588-1603.
42. J.-M. Joubert et al. Assessment of the niobium–nickel system, *Calphad* 28 (3) (2004) 299–306
43. T. Keller et al., Application of finite element, phase-field, and calphad-based methods to additive manufacturing of ni-based superalloys, *Acta Materialia* 139 (2017) 244–253.
44. M. v. Pantawane et al. Spatial Variation of Thermokinetics and Associated Microstructural Evolution in Laser Surface Engineered IN718: Precursor to Additive Manufacturing. *Metallurgical and materials transactions a* 2344—volume 52a, june 2021.
45. T. Mukherjee et al. Heat and fluid flow in additive manufacturing – Part II: Powder bed fusion of stainless steel, and titanium, nickel and aluminum base alloys. *Computational Materials Science* 150 (2018) 369–380
46. P. Mohammadpour and A. B. Phillion. Solidification microstructure selection maps for laser powder bed fusion of multicomponent alloys. *IOP Conf. Series: Materials Science and Engineering* 861 (2020) 012005
47. A. T. Polonsky et al. Scan strategies in EBM-printed IN718 and the physics of bulk 3D microstructure development [Author links open overlay panel](#). *Materials Characterization* Volume 190, August 2022, 112043.
48. J. Zhang et al. Research on the evolution mechanism of solidified structure during laser cladding IN718 alloy. *Applied Thermal Engineering*. Volume 215, October 2022, 118925.
49. J.D. Hunt, Steady state columnar and equiaxed growth of dendrites and eutectic, *Materials Science and Engineering* Volume 65, Issue 1, July 1984, Pages 75-83.
50. J. Hunt. Cellular and primary dendrite spacings. In: *Solidification and casting of metals*. Proc. Conf, Sheffield, England (1979).
51. Y. Lee et al. Effect of fluid convection on dendrite arm spacing in laser deposition. 2014 *Metall. Mater. Trans. B* 45(4) 1520-9
52. M. Gaumann et al. Single-crystal laser deposition of superalloys: processing–microstructure maps, *Acta Materialia* 49(6) (2001) 1051-1062
53. A. Reza Ansari Dezfoli et al. Prediction of Epitaxial Grain Growth in Single-Track Laser Melting of IN718 Using Integrated Finite Element and Cellular Automaton Approach. *Materials*, 14, 5202, 2021.
54. Y. Lin, L. Zheng. Marangoni boundary layer flow and heat transfer of copperwater nanofluid over a porous medium disk. *AIP ADVANCES* 5, 107225 (2015).

55. J. I. Arrizubieta et al. Evaluation of the relevance of melt pool dynamics in Laser Material Deposition process modeling. International Journal of Heat and Mass Transfer 115 (2017) 80–91.
56. V.R. Voller and C. Prakash, A fixed grid numerical modeling methodology for convection — diffusion mushy region phase-change problems, Int.J.Heat Mass Transfer, vol. 30, pp. 1709–1719, 1987.
57. A.D. Brent. Enthalpy-Porosity Technique for Modeling Convection-Diffusion Phase-Change—Application to the Melting of a Pure Metal. Numer. Heat Transf. 1988, 13, 297–318.
58. Bo Chen et al. Effect of Laser Beam Profile on Thermal Transfer, Fluid Flow and Solidification Parameters during Laser-Based Directed Energy Deposition of Inconel 718. Materials 2023, 16, 4221.
59. Continuous Casting. COMSOL example. Available from: <https://www.COMSOL.com/>
60. Jayasimha SLN, N L Murali Krishna, H.P. Raju. Development of semi-empirical model to estimate surface finish of Inconel-625 alloy in extrusion honing process. Results in Engineering 15 (2022) 100575.
61. Akash Aggarwal et al. Role of impinging powder particles on melt pool hydrodynamics, thermal behaviour and microstructure in laser-assisted DED process: A particle-scale DEM – CFD – CA approach. International Journal of Heat and Mass Transfer 158 (2020) 119989
62. S. Ghosh et al, On the primary spacing and microsegregation of cellular dendrites in laser deposited Ni–Nb alloys. Modelling Simul. Mater. Sci. Eng. 25 (2017) 065002.
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Appendix A

Parameters

Table A1. List of the DED simulation parameters for INCONEL 625 (Ref. 60–62)

Parameters and units	Value
Solid density, ρ , kg/m^3	8440
Solidus temperature, T_S , K	1563
Liquidus temperature, T_L , (K)	1623
Latent heat of fusion, L_f kJ/kg	290
Dynamic viscosity, μ (Pas-s)	$7 \cdot 10^{-3}$
Specific Heat Capacity, C_p , J/kgK	709
Cladding velocity v_0 , m/s	0.005-0.1
Thermal expansion coefficient, β 1/K	$\sim 5 \cdot 10^{-7}$
Surface tension, σ N/m	1.8
Convection Coefficient $W/m^2.K$	10

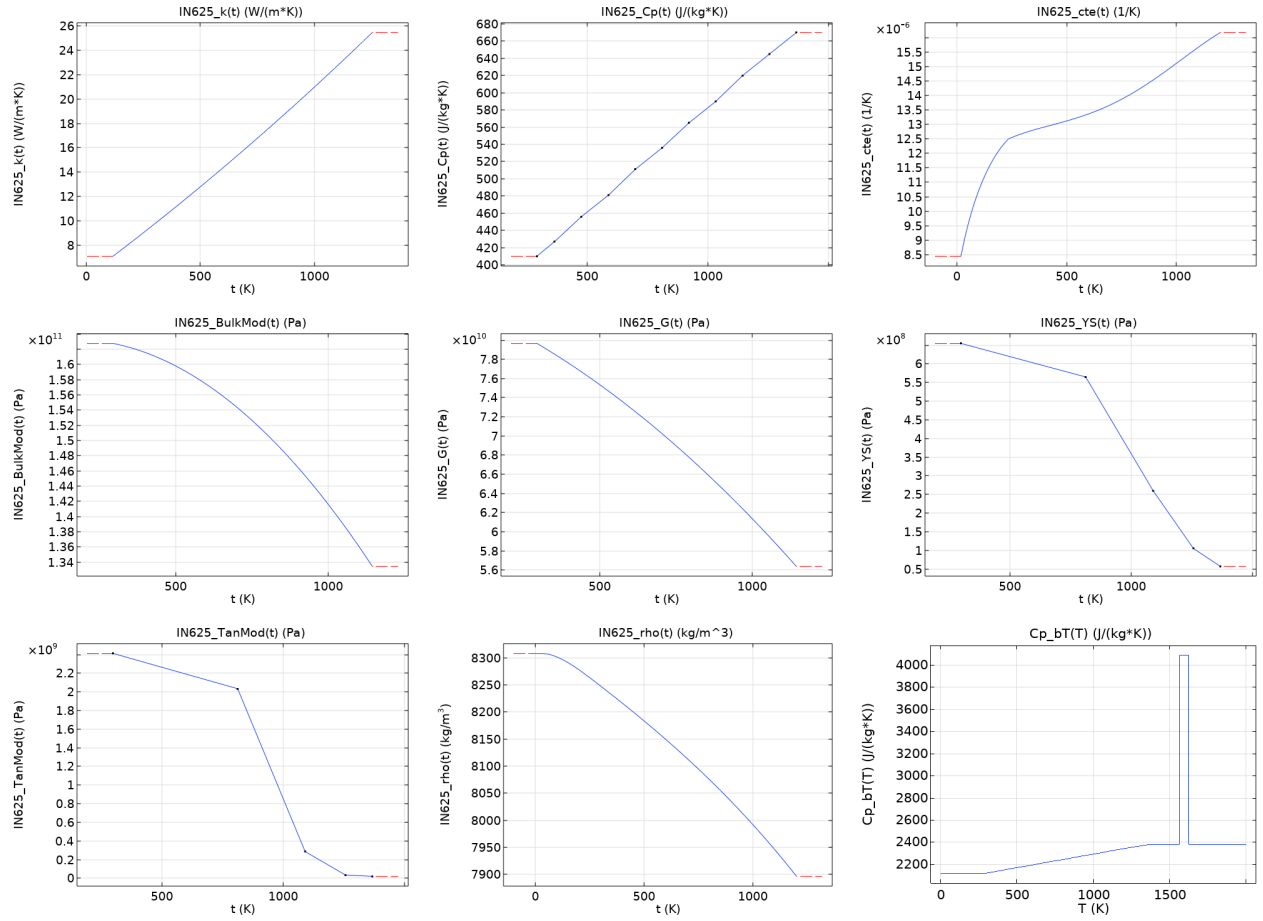


Figure A62.—Material parameter temperature dependencies for INCONEL 625 that used for simulations (Ref. 60–62)

Table A2. Process parameters of DED for INCONEL 625

Parameters of INCONEL 625 used for PDAS microstructure calculation

Parameter,	value	units	Ref	
Liquidus slopes, m_{Nb} ,	-1199	K/m	(Ref. 46, 51, 62)	
Partition coefficients, k_{Nb}	0.5		(Ref. 46, 51, 62)	
Gibbs-Thomson coefficient, Γ	$3.6 \cdot 10^{-7}$	m/K	(Ref. 46, 51, 62)	
Diffusion coefficient in the liquid, D_l	$3 \cdot 10^{-9}$	m^2/s	(Ref. 46, 51, 62)	
Nucleation undercooling of equiaxed grains, ΔT	1.5	K	(Ref. 46, 51, 62)	
Nucleation density of equiaxed grains, N_0	$1/m^3$	10^{15}	(Ref. 46, 51, 62)	
