



Mechanism of crystallographic lamellar microstructure formation in PBF-LB 316L stainless steel: A numerical simulation study

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ABSTRACT

In this study, finite element thermal simulations were coupled with ExaCA, a cellular automaton model for microstructure evolution, to investigate the solidification behavior of SS316L fabricated by powder bed fusion by laser beam (PBF-LB) under different laser conditions and to elucidate the formation mechanism of crystallographic lamellar microstructure (CLM). A heat transfer model was employed to accurately capture melt pool geometry, and the resulting thermal data were then used as input for ExaCA to simulate microstructure evolution. The framework successfully reproduced both the melt pool geometry and the experimentally observed texture, thereby providing a simulation-validated basis for mechanistic analysis rather than relying solely on inference from experimental observations. The results reveal that the major $\langle 110 \rangle // Z$ layer, where Z denotes the build direction, is governed by the thermal gradient direction in the overlap region near the melt pool bottom, which promotes coherent epitaxial growth of mutually perpendicular dendrites across adjacent tracks. In contrast, the minor $\langle 100 \rangle // Z$ layer is controlled by the distribution of the thermal gradient components along the transverse (Y) and build (Z) directions near the center of the melt pool bottom, where a sufficiently low lateral gradient enables epitaxial growth along the build direction. These findings demonstrate that CLM formation is governed by the directional distribution of thermal gradients near the melt pool bottom rather than simply by the overall melt pool shape, providing a mechanistic basis for understanding and controlling texture development in materials fabricated by powder bed fusion.

1. Introduction

Additive manufacturing (AM) technologies, particularly powder bed fusion by laser beam (PBF-LB), fabricate components through layer-by-layer melting of metallic powders. Compared with conventional manufacturing processes, PBF-LB offers significantly greater geometric design freedom and has consequently attracted considerable attention in industries with demanding requirements for component complexity, such as aerospace, energy, and biomedical engineering [1–4]. Unlike conventional processes, PBF-LB is characterized by extremely high temperature gradients and rapid cooling rates (up to 10^6 K/s), which substantially suppress elemental segregation while simultaneously introducing elevated dislocation densities [5]. These distinctive thermal conditions result in microstructures that are fundamentally different from those obtained through conventional processing routes. Stainless steel (SS) alloys, such as SS316L, have been extensively investigated for

PBF-LB applications due to their excellent solidification behavior, which is primarily attributed to the high solid solubility among the three principal constituents: Fe, Ni, and Cr [6]. Furthermore, SS316L can be processed to near-full density over a relatively broad PBF-LB processing window, in which solidification cracking is absent and porosity remains minimal; thus, the influence of defects is minimized [7].

Previous studies have demonstrated that materials fabricated by PBF-LB can exhibit a superior combination of strength and ductility at room temperature compared with their conventionally cast or wrought counterparts [8–10]. This enhancement is closely associated with the non-equilibrium microstructural evolution driven by steep temperature gradients, rapid solidification, and repeated thermal cycling [11]. While early research efforts predominantly focused on optimizing processing parameters to achieve full density and minimize defects [12,13], increasing attention has been directed toward understanding how the thermal conditions within the melt pool govern microstructural

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development, particularly grain orientation selection. Since PBF-LB is inherently a solidification-dominated process, the local heat flow direction within the melt pool plays a critical role in determining the crystallographic orientation of the resulting grains [14]. Moreover, partial remelting of the previously solidified material and steep thermal gradients in PBF-LB often lead to epitaxial grain growth from the underlying substrate [15]. During epitaxial growth, dendrites preferentially grow along their preferred crystallographic directions; therefore, the spatial distribution and directionality of the temperature gradient within the melt pool directly govern the grain orientation selection and competitive growth behavior [16]. Furthermore, the thermal gradient magnitude and solidification velocity collectively determine the solidification morphology, while the cooling rate controls the dendrite arm spacing [17,18]. These relationships establish a direct link between PBF-LB processing conditions and the resulting grain morphology and crystallographic texture. It is thus evident that PBF-LB not only provides geometric design freedom but also offers the potential to engineer mechanical properties through deliberate microstructural control [19–21].

Extensive efforts to control crystallographic texture through PBF-LB have successfully produced single-crystal-like and fiber-type textures in a variety of metallic alloy systems [22–24]. Sun et al. further discovered that under appropriate processing parameters and scanning strategies, PBF-LB can yield alloys with a unique lamellar structure [25]. Conventional lamellar structures typically consist of multilayered microstructures composed of distinct phases; however, this newly identified lamellar structure comprises alternating layers of the same phase but with different crystallographic orientations, and is therefore termed the crystallographic lamellar microstructure (CLM) [25–27]. Relative to the build direction, the wider major layers and narrower minor layers are oriented along the $\langle 110 \rangle$ and $\langle 100 \rangle$ directions, respectively. It should be noted that the CLM is distinct from the nanoscale cellular substructure, such as the dislocation cells and solute-segregation cells that develop within individual grains. The cellular substructure arises from solute redistribution on the scale of the cell or dendrite arm spacing, whereas the CLM refers specifically to a grain-scale lamellar arrangement in which adjacent layers differ in crystallographic orientation. The two features therefore originate from different physical processes acting on different length scales, and the present work is concerned with the latter. Studies have also indicated that materials possessing the CLM exhibit superior mechanical properties, thereby attracting widespread research interest [25,26,28]. Notably, the CLM has been observed not only in SS316L but also in other alloy systems, suggesting that the CLM is a general phenomenon associated with the PBF-LB solidification process rather than being specific to a particular material. Nevertheless, the existing literature has predominantly attempted to explain CLM formation from the perspective of experimentally observed melt pool morphology, while systematic verification through numerical simulation remains lacking [29]. This gap hinders the ability to precisely control and engineer the CLM through process parameter optimization.

To overcome the limitations of purely experimental approaches, numerical simulation has emerged as a powerful complementary tool for investigating solidification microstructures in PBF-LB. Modeling of solidification processes in PBF-LB is typically conducted at two scales: the individual dendrite scale and the grain scale. Among the various modeling approaches, the phase field (PF) method, which is based on rigorous free energy formulations, can accurately describe interface evolution [30–32]; however, its prohibitively high computational cost limits the spatial extent of the microstructure that can be predicted. In contrast, the cellular automaton (CA) model, which operates through defined transition rules, cell states, and interactions between neighboring cells, can efficiently simulate nucleation, grain growth, and competitive solidification processes, thereby providing grain-scale visualization of microstructural evolution [33–36]. Furthermore, melt pool geometry, such as that observed in conduction mode versus keyhole mode, profoundly influences the temperature gradient distribution. To accurately capture the transient temperature field evolution

during the PBF-LB process, the finite element method (FEM) has been widely adopted as a thermal solver owing to its capability to resolve the steep temperature gradients and rapid heating-cooling cycles characteristic of laser-material interactions [37,38]. When the CA model is coupled with FEM thermal simulation, the resulting FEM-CA framework enables the prediction of multi-layer, multi-track microstructural evolution under physically meaningful thermal boundary conditions [35, 39,40]. Despite these advances, simulation studies specifically targeting the formation mechanism of CLM remain scarce. Although attempts have been made to reproduce CLM through a PF-based approach [41], the minor $\langle 100 \rangle$ //Z layer was not fully captured due to the limitations of the Gaussian heat source model employed. A simulation that reproduces the CLM and elucidates its formation mechanism has yet to be achieved.

In this study, a coupled FEM-CA simulation framework is employed to simulate the solidification microstructural evolution of SS316L in the PBF-LB process. The temperature distribution within the melt pool is obtained through FEM and subsequently imported into the ExaCA model to predict the resulting grain structure. By quantifying the thermal gradient direction near the melt pool bottom and by examining the interaction between adjacent melt pools in the overlap region, this study aims to elucidate the formation mechanism of the CLM, thereby providing a deeper theoretical foundation for the precise control of microstructure in future applications.

2. Materials and methods

2.1. Experimental procedure

Gas-atomized SS316L powder was used in this study. The particle size distribution exhibited D_{10} , D_{50} , and D_{90} values of 19.3, 31.5, and 51.3 μm , respectively. The chemical composition of the powder is listed in Table 1. Cubic specimens with dimensions of $10 \times 10 \times 13 \text{ mm}^3$ were fabricated for microstructural characterization using an SLM280 HL system (SLM Solutions, Germany), equipped with a Gaussian laser with a spot radius of 40 μm .

The processing parameters included a substrate preheating temperature of 200 °C, a layer thickness of 40 μm , a hatch spacing of 80 μm , and a bidirectional back-and-forth scanning strategy with a 0° interlayer rotation. The directions parallel and transverse to the laser scan vectors are defined as the X and Y directions, respectively, while the build direction is designated as the Z direction. Specimens were fabricated using various combinations of laser power and scan speed. Based on preliminary optimization, a constant scan speed of 1000 mm/s with three different laser powers (150 W, 250 W, and 350 W) was selected for systematic comparison.

The as-built samples were sectioned along the center plane using a low-speed diamond saw to expose the YZ cross-section, followed by standard metallographic grinding and polishing procedures. To reveal the melt pool morphologies, the polished surfaces were etched in aqua regia ($\text{HCl}:\text{HNO}_3 = 3:1$ by volume) for approximately 50 s. Microstructural observations were performed using an optical microscope (OM, KEYENCE VHX-7000) and a field-emission scanning electron microscope (FE-SEM, JSM-7900F, JEOL). Crystallographic orientation and grain morphology were characterized by inverse pole figure (IPF) maps obtained from electron backscatter diffraction (EBSD) analysis.

Table 1
Chemical composition of SS316L powder.

Composition in wt.%								
Fe	Mo	Si	Cr	Ni	Mn	N	C	O
Bal.	2.51	0.51	16.84	11.08	0.69	0.056	0.017	0.05

2.2. FEM-CA simulation framework

2.2.1. General overview

Fig. 1 illustrates the simulation framework adopted in this study. First, the transient temperature field induced by a single-track laser scan is computed using the FEM, and the nodal thermal histories are extracted. The single-track thermal field is then duplicated and spatially translated to reconstruct the desired multi-track, multi-layer scanning strategy. The resulting temperature data are subsequently provided as input to the ExaCA framework to simulate grain solidification during the PBF-LB process. At the beginning of each layer, a powder layer with a prescribed thickness and randomly assigned crystallographic orientations is deposited onto the previously solidified microstructure. The laser melting process is then simulated based on the reconstructed thermal field, and this layer-by-layer procedure is repeated until the predefined number of layers is completed.

2.2.2. FEM thermal simulation

To elucidate the relationship between laser parameters and melt pool behavior, and to provide thermal input data for ExaCA simulations, a three-dimensional thermal model was developed using Abaqus/Standard to simulate the temperature evolution during single-track laser scanning. The computational domain consisted of a cubic volume with an edge length of 300 μm , discretized with a uniform element size of 5 μm . A uniform initial temperature of $T_0 = 573$ K was applied to the domain. The resulting thermal data were subsequently interpolated onto a finer grid with a 1 μm spacing for use as input to ExaCA; the thermal gradient and solidification velocity analyzed in Section 2.3 were evaluated on the original 5 μm nodes. A moving volumetric laser heat source, implemented via a user-defined DFLUX subroutine, was employed to capture the transient melt pool dynamics. The heat source traveled along the X direction across the surface of the SS316L substrate, enabling simulation of the temperature distribution associated with a single laser track. The thermophysical properties of SS316L used in the model were adopted from the literature [42] and are summarized in Fig. 2. Above the melting point the property set of [42] specifies an elevated thermal conductivity, which that work adopts in order to represent the enhanced heat transfer produced by fluid flow and thermocapillary convection in the weld pool without resolving the flow field; it is therefore an effective rather than a physical transport coefficient, and because the tabulated values are interpolated linearly it is already partially active within the solidification interval. The liquidus and solidus temperatures were taken as $T_L = 1673$ K and $T_S = 1643$ K, T_L corresponding to the melting point at which that property set switches to its liquid values. The latent heat of fusion was not included in the present calculation.

The transient three-dimensional temperature field was obtained by solving the governing heat conduction equation:

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

where ρ ($\text{kg} \cdot \text{m}^{-3}$), C_p ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$), and λ ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$) refer to material density, specific heat capacity, and thermal conductivity, respectively. T (K) is system temperature, t (s) denotes time and Q ($\text{W} \cdot \text{m}^{-3}$) is the volumetric internal heat generation.

The heat input at a material point located at $(\Delta x, \Delta y, \Delta z)$ relative to the center of a laser beam moving at a velocity v ($\text{m} \cdot \text{s}^{-1}$) with laser power P (W) is modeled using a three-dimensional super-Gaussian volumetric heat source model [43]. The volumetric heat generation term Q_{heat} is given by:

$$Q_{\text{heat}} = \frac{\eta P}{V_0} \exp \left(- \left[\left(\frac{\Delta x}{r(z)} \right)^2 + \left(\frac{\Delta y}{r(z)} \right)^2 \right]^{k/2} \right) \quad (2)$$

where η (dimensionless) is the laser absorptivity, V_0 (m^3) is the volume integral of the heat source distribution and k (dimensionless) is the Gaussian exponent controlling the lateral heat distribution. The attenuation of the heat source intensity along the depth direction (z -direction) is governed by the decay of the radius $r(z)$ (m):

$$r(z) = \frac{r_0}{\sqrt[k]{2}} \left(1 - \left| \frac{\Delta z}{d} \right|^m \right)^{1/m} \quad (3)$$

where r_0 (m) is the laser spot radius, d (m) is the heat source depth and m (dimensionless) is a volumetric shape parameter. The Macaulay brackets $\langle \cdot \rangle$ ensure that the heat source is confined within the prescribed depth.

The employed heat source model is formulated to achieve a balance between the physical fidelity necessary for accurate prediction of melt pool size and morphology with the need for computational efficiency [43]. To this end, the model is based on the heat conduction equation, and does not resolve the melt pool flow field or represent the discrete powder feedstock, as these phenomena dominate the computational cost in melt pool-scale simulations. Rather than resolving these effects directly, the laser energy input is represented by an effective volumetric heat source distribution, and the heat transport associated with melt pool convection is represented in an effective manner through the elevated liquid-phase thermal conductivity described above. To account for the experimentally observed transition from conduction-mode melting to keyhole-mode melting, which is characterized by a pronounced increase in melt pool depth and aspect ratio, the heat source depth is dynamically adjusted. Recent studies have established quantitative relationships between the normalized melt pool depth $d^* = d/r_0$, a dimensionless parameter β_η (referred to as the Keyhole number or normalized enthalpy and dependent on η), and the normalized thermal diffusion length L_{th}^* [44–46]:

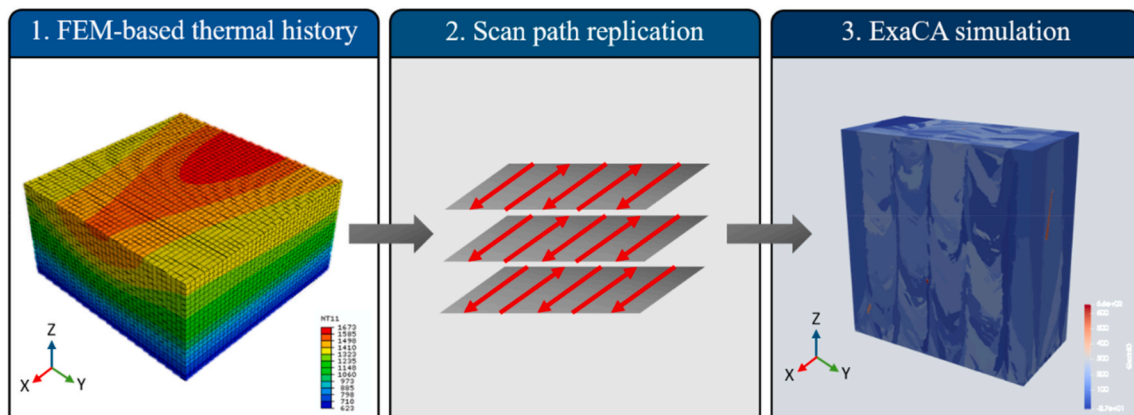


Fig. 1. Schematic illustration of the numerical simulation framework adopted in this study.

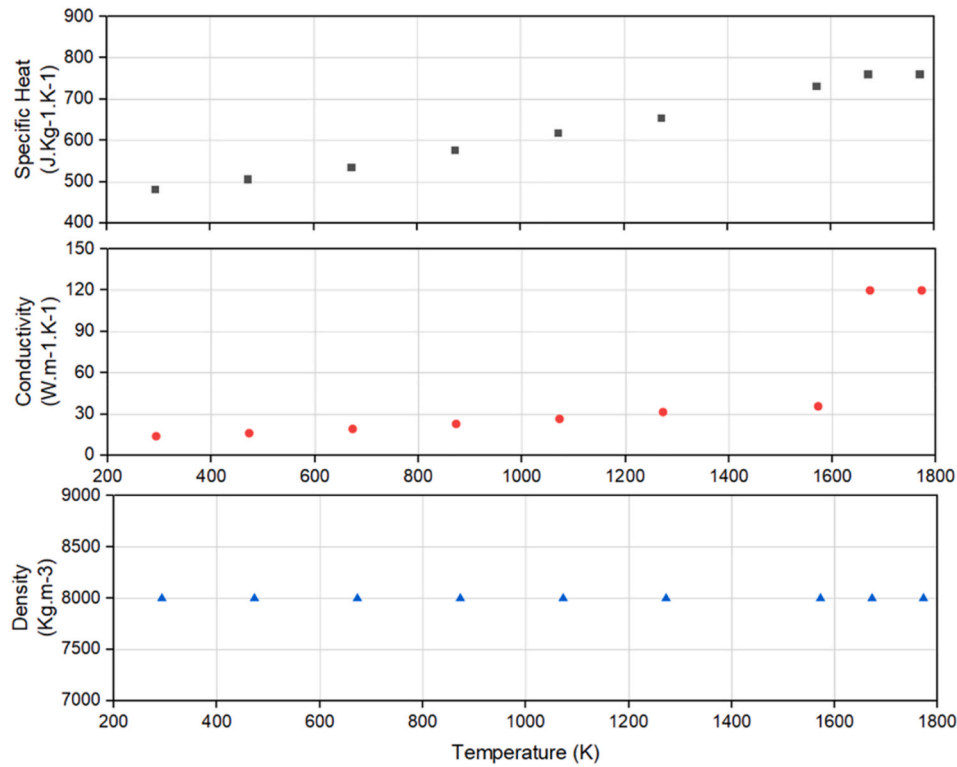


Fig. 2. Thermophysical properties of SS316L taken from literature [42].

$$d^* = \frac{d}{r_0} = 0.6\beta_\eta L_{th}^* = 0.6 \left(\frac{\eta P}{\pi h_s \sqrt{\kappa \nu (r_0)^3}} \right) \sqrt{\frac{\kappa}{\nu (r_0)}} \quad (4)$$

where $h_s = \rho C_p (T_m - T_0)$ ($J \cdot m^{-3}$) represents the enthalpy at melting, with T_m (K) and T_0 (K) denoting the melting and the initial temperatures, respectively, and κ ($m^2 \cdot s^{-1}$) being the thermal diffusivity. To further incorporate a physically informed description of the absorptivity evolution across different melting regimes, a two-parameter absorptivity model expressed as a function of d^* is employed:

$$\eta = \begin{cases} \eta_c & \text{if } \frac{d}{r_0} \leq 1 \\ \eta_k (1 - e^{-0.66\beta_{\eta_k} L_{th}^*}) & \text{if } \frac{d}{r_0} > 1 \end{cases} \quad (5)$$

where η_c and η_k (dimensionless) correspond to the laser absorptivity in the conduction and keyhole melting modes, respectively. The determination of the heat source depth d and absorptivity η follows an iterative procedure. First, the normalized melt pool depth d^* is evaluated using Eq. (4) with an initial absorptivity of η_c . If the resulting $d^* \leq 1$, the conduction-mode absorptivity η_c is retained; otherwise, the absorptivity is updated to the keyhole-mode value using Eq. (5), and d^* is recalculated accordingly. This procedure ensures a self-consistent determination of both d and η for each set of laser parameters. Based on literature reports, η_c and η_k are set to 0.35 and 0.7 in this study [43,47,48]. The heat source shape parameters k and m were selected based on prior literature and calibrated against experimentally observed melt pool geometries [43,47]. Specifically, $k = 2$, corresponding to a Gaussian lateral heat distribution, and $m = 6$ were adopted in the present simulations.

Heat loss (Q_{loss} , $W \cdot m^{-2}$) from the material surface to the surrounding environment through radiation and natural convection is described by the following boundary condition:

$$Q_{loss} = \sigma_B \epsilon (T^4 - T_{amb}^4) + h(T - T_{amb}) \quad (6)$$

where ϵ (dimensionless) is the emissivity taken as 0.3, σ_B is the Stefan-Boltzmann constant ($5.67 \times 10^{-8} W \cdot m^{-2} \cdot K^{-4}$), T_{amb} denotes the ambient temperature (473 K), and h is the convective heat transfer coefficient ($20 W \cdot m^{-2} \cdot K^{-1}$). The two temperatures appearing above should be distinguished. T_{amb} corresponds to the substrate preheating temperature used experimentally. T_0 of the computational domain is higher than this and represents the heat accumulation that develops during the build. Heat accumulation during PBF-LB has been shown to raise the temperature of previously deposited material [49], but its magnitude depends on factors such as the inter-layer dwell time and the heat extraction path toward the baseplate, and cannot therefore be prescribed directly. The value adopted here was determined by calibration against the experimentally measured melt pool dimensions; a single value was used for all three laser power conditions and is therefore constrained by the complete set of measured melt pool dimensions rather than adjusted for each condition.

2.2.3. CA microstructure simulation

In this study, the open-source CA-based software ExaCA was employed to predict solidification microstructure evolution during additive manufacturing [50,51]. ExaCA incorporates the key physical mechanisms governing grain structure evolution and texture development during dendritic solidification of metallic alloys under additive manufacturing conditions. The first mechanism is heterogeneous nucleation of new grains within the undercooled liquid ahead of the solidification front. The second is the solidification kinetics of grains at the solid-liquid interface. Within the CA framework, the computational domain is discretized into a regular array of cells, each of which is assigned a state corresponding to liquid, solid, or active, where the active state represents cells located at the solidification front. The state of each cell is updated according to predefined transition rules based on the thermal history and neighboring cell states. The local solidification velocity of a grain is governed by an approximate relationship known as the interfacial response function, which expresses V ($m \cdot s^{-1}$) as a power-law function of the local undercooling ΔT (K) within a cell [52]:

$$V(\Delta T) = A(\Delta T)^B \quad (7)$$

where A ($\text{m}\cdot\text{s}^{-1}\cdot\text{K}^{-B}$) and B (dimensionless) are fitting parameters. In this study, the values of A and B for SS316L were taken from the default parameter set provided in the ExaCA repository. The complex dendritic growth morphology is phenomenologically approximated by a regular octahedral envelope whose vertices are aligned with the preferred $\langle 100 \rangle$ crystallographic growth directions. A liquid cell is converted to a solid state when its center becomes enclosed by the advancing fronts of neighboring growing grains. To minimize artificial growth anisotropy induced by the underlying computational grid, an eccentric octahedron algorithm is employed, which effectively suppresses preferential growth along grid-aligned directions [34].

CA simulations were performed to predict microstructure formation under processing conditions identical to those used in the experiments. The simulations were conducted within a rectangular computational domain in the XY plane with in-plane dimensions of $200 \times 460 \mu\text{m}^2$ and a cell size of $1 \mu\text{m}$. At the beginning of each layer, a powder layer composed of randomly sampled crystallographic orientations was deposited onto the previously solidified microstructure. The transient thermal field obtained from the single-track laser simulation served as input to the CA model. Specifically, the spatial coordinates of cells exceeding the melting temperature, along with their corresponding melting and solidification times and cooling rates, were extracted from the thermal simulation. These thermal data were then duplicated and translated to reproduce the experimental scanning strategy. Each simulation comprised a total of 20 deposited layers. The parameters employed in the CA simulations are summarized in Table 2. In the present simulations, the nucleation density was set to zero to suppress stochastic variability arising from randomly nucleated grains. This assumption is consistent with prior CA-based studies of additive manufacturing, in which heterogeneous nucleation is commonly neglected under the large thermal gradients characteristic of melt pool solidification, where epitaxial grain growth is expected to dominate [15, 53, 54]. The validity of this assumption is assessed in Section 4.3.

2.3. Quantitative analysis

To quantitatively characterize the solidification conditions within the melt pool and the resulting crystallographic texture, several key quantities were extracted from the FEM thermal simulation and the CA microstructure simulation.

The cooling rate $\dot{T}$ ($\text{K}\cdot\text{s}^{-1}$) was determined by analyzing the temporal evolution of the nodal temperature history. For each node that experienced melting, the time at which the temperature decreased to the liquidus temperature, t_m , and the time at which it further decreased to the solidus temperature, t_s , were identified. The cooling rate was then calculated as the average rate of temperature change over the solidification interval:

$$\dot{T} = \left| \frac{T_L - T_S}{t_s - t_m} \right| \quad (8)$$

Equation (8) therefore defines an interval-averaged cooling rate, rather than an instantaneous rate. The interval-averaged value is used because

it characterizes the thermal condition experienced by the growing dendrite over the entire course of solidification, which is the quantity relevant to the growth-direction selection analyzed here.

The solidification velocity R was obtained by analyzing the spatial distribution of the solidification arrival time t_s . For each melted node in the original $5 \mu\text{m}$ spacing grid, the eight nearest nodes with valid solidification times were identified by a nearest-neighbor search; nodes near the boundary of the melted region, for which fewer than four neighboring nodes had valid solidification times, were excluded. These comprise the six face-adjacent nodes, together with two of the twelve edge-adjacent nodes. A three-dimensional linear model of the solidification time was then fitted by least squares, giving the gradient vector of the solidification time field:

$$\nabla t_s = \left(\frac{\partial t_s}{\partial x}, \frac{\partial t_s}{\partial y}, \frac{\partial t_s}{\partial z} \right) \quad (9)$$

The solidification velocity in the normal direction was subsequently determined as the reciprocal of the magnitude of this gradient:

$$R = \frac{1}{\|\nabla t_s\|} \quad (10)$$

which represents the propagation speed of the isothermal surface along its local normal direction.

The thermal gradient G ($\text{K}\cdot\text{m}^{-1}$) was derived from the coupling relationship between the cooling rate and the solidification velocity. Since the thermal gradient is directed along the local normal of the solidification front, its vector form is expressed as:

$$G = \frac{\dot{T}}{R} \hat{n} = \frac{\dot{T}}{R} \frac{\nabla t_s}{\|\nabla t_s\|} = \dot{T} \nabla t_s \quad (11)$$

where $\hat{n}$ is the unit normal vector of the solidification front.

To characterize the orientation of the thermal gradient with respect to the build direction, the angle between the thermal gradient vector and the Z-axis was evaluated on the YZ cross-section. Since the X-component of the thermal gradient is comparatively small on this plane and does not significantly affect the angular distribution, the angle was calculated using the ratio of the Y- and Z-components of the thermal gradient:

$$\theta = \tan^{-1} \left(\frac{|G_y|}{|G_z|} \right) \quad (12)$$

where G_y and G_z denote the Y- and Z-components of the thermal gradient vector, respectively. A value of $\theta = 0^\circ$ indicates that the thermal gradient is aligned with the build direction, while $\theta = 90^\circ$ corresponds to a purely lateral gradient directed along the Y-axis.

3. Results

3.1. Thermal simulation

To observe the complete melt pool morphology and dimensions under different processing conditions, OM was employed to examine etched YZ plane sections taken from the top region of the specimens. The observed melt pool profiles were superimposed with the corresponding simulated results, as shown in Fig. 3(a–c), and the quantitative measurements are summarized in Fig. 3(d). Distinct melt pool boundaries are clearly visible in all images. The melt pool dimensions were characterized by measuring the top-surface width, the width at half depth, and the depth measured downward from the nominal flat surface. Multiple melt pools were measured for each processing condition to obtain statistically representative values. At a constant scan speed, increasing laser power resulted in a systematic increase in all melt pool dimensions, with the width exhibiting a more pronounced increase than the depth. This trend is consistent with observations reported in the literature, where higher incident energy promotes multiple laser

Table 2
CA simulation parameters.

Parameter	Value
Cell size (μm)	1
Interfacial response, A. ($\text{m}\cdot\text{s}^{-1}\cdot\text{K}^{-B}$)	7.33×10^{-6}
Interfacial response, B. (–)	3.12
Nucleation density, main simulations. (m^{-3})	0
Nucleation density, sensitivity analysis. (m^{-3})	1×10^{15}
Mean nucleation undercooling (K)	5
Std. dev. of nucleation undercooling (K)	0.5

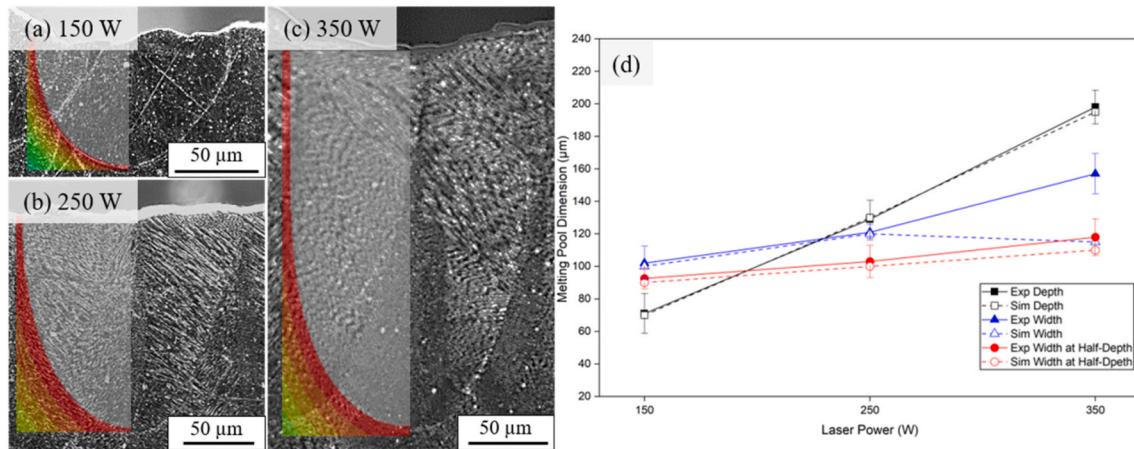


Fig. 3. Cross-sectional OM images overlaid with the corresponding simulated melt pool dimensions under (a) 150 W, (b) 250 W, and (c) 350 W conditions. (d) Quantitative comparison between simulated and experimentally measured melt pool dimensions.

reflections within the melt pool cavity and facilitates a transition toward keyhole-mode melting, leading to deeper and more elongated melt pool geometries [47].

The simulated melt pool profiles successfully capture the overall morphology observed experimentally and exhibit good quantitative agreement in terms of characteristic dimensions. Although the simulated top-surface width is slightly smaller than the experimental value under 350 W condition, the width at half depth exhibits excellent agreement. This level of consistency in the lower part of the melt pool is considered sufficient for subsequent analyses, particularly those related to thermal gradient and solidification behavior.

3.2. Microstructure simulation

Fig. 4 presents etched melt pool boundaries under different processing conditions (Fig. 4(a–c)) together with IPF-colored EBSD maps (Fig. 4(d–f)).

along the build direction (Fig. 4(d–f)). After etching, regularly arranged melt pools are clearly observed, with unremelted regions present at the bottom of each melt pool. Adequate overlap is evident both between adjacent tracks and between successive layers, confirming complete melting and the absence of lack-of-fusion defects under all investigated conditions. Notably, a distinct region extending continuously across multiple melt pools from the central area is observed only under the 250 W condition. This feature suggests a localized and persistent solidification characteristic unique to this condition.

The EBSD maps reveal pronounced differences in microstructural morphology as a function of laser power. At 150 W, the microstructure is characterized by fine, polycrystalline grains with no apparent preferred orientation. Under 250 W, a CLM that is reported in the literature is observed. The CLM consists of alternating layers of grains with two distinct crystallographic orientations: a major layer aligned with the $\langle 110 \rangle // Z$ direction and a minor layer aligned with the $\langle 100 \rangle // Z$

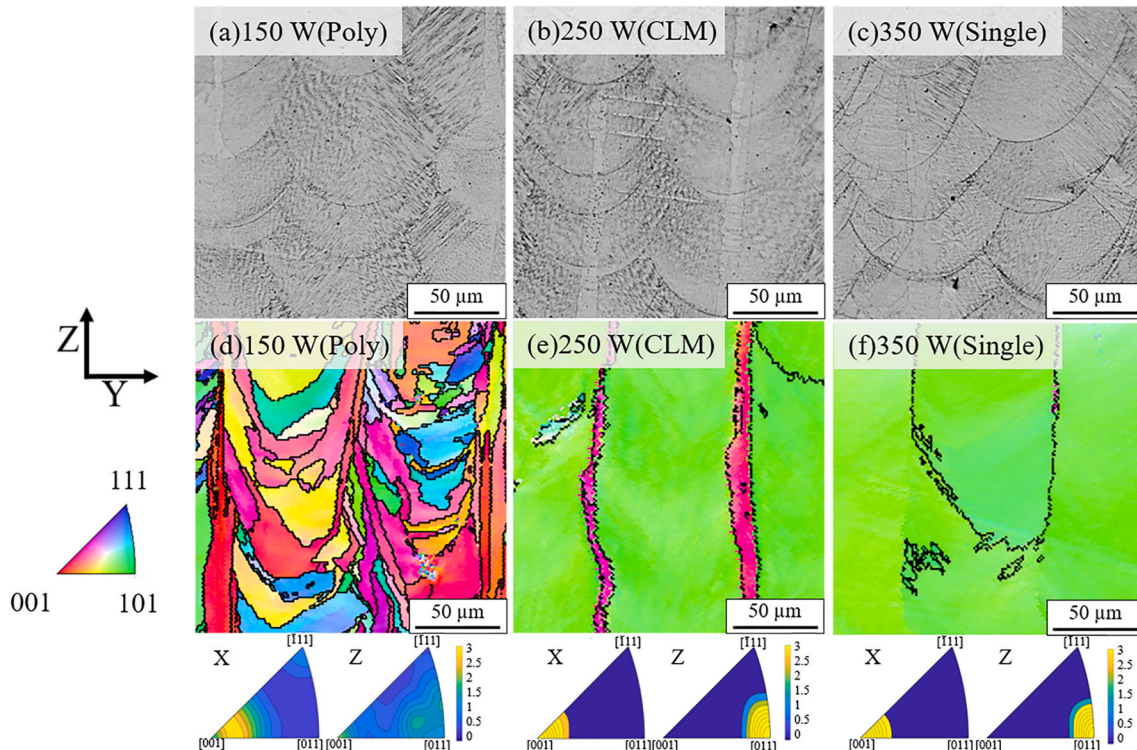


Fig. 4. Experimental OM images (a–c) and IPF-Z maps (d–f) obtained under different processing conditions: (a, d) 150 W, (b, e) 250 W, and (c, f) 350 W.

direction. At the highest laser power of 350 W, the microstructure evolves toward a nearly single-crystalline structure, with grains predominantly exhibiting the $\langle 110 \rangle // Z$ orientation across multiple layers.

Fig. 5(a–c) present the ExaCA simulation results obtained under identical laser processing conditions, while Fig. 5(d–f) display the corresponding two-dimensional EBSD maps on the upper YZ plane, colored according to IPF color coding along the build direction. Given that grain competition at the domain boundaries is spatially constrained, the edge regions are not fully representative of the bulk microstructure; therefore, the analysis focuses primarily on the central region. The fine-grained zone at the bottom of each map corresponds to the preset substrate layer. A progressive microstructural transition is clearly observed with increasing number of simulated layers, reflecting the gradual evolution of grain morphology driven by competitive growth along the thermal gradient direction. This observation is consistent with findings reported in the literature [55]. Furthermore, the two-dimensional cross-sections confirm that the CA simulations accurately capture the microstructural variations associated with changes in laser processing conditions. These results indicate that the heat source model reproduces the melt pool geometry and the grain structure that develops from it.

Accordingly, a thermal gradient analysis of the melt pool was conducted based on the thermal field described above. The cooling rate, solidification velocity, and thermal gradient vector at each node were calculated following the procedures described in Section 2.3. As illustrated in Fig. 6, the thermal gradient distributions within the melt pool on the YZ cross-section are presented for the three processing conditions. In addition to the expected differences in melt pool dimensions, the highest thermal gradient magnitudes are predominantly concentrated near the bottom of the melt pool. Moreover, the thermal gradient vectors are generally oriented normal to the melt pool boundary, transitioning from a vertically upward orientation at the melt pool bottom to a nearly horizontal direction pointing toward the melt pool center along the lateral sides.

4. Discussion

4.1. Crystallographic origin of major $\langle 110 \rangle // Z$ layer

To elucidate the origin of the layered microstructure, the simulation results reveal that the major $\langle 110 \rangle // Z$ layer is governed by the thermal gradient direction specifically within the bottom unremelted region of the melt pool, where epitaxial continuity is established across neighboring tracks. As illustrated in Fig. 4(a–c), the PBF-LB material is built through successive laser melting of individual scan tracks, in which only the bottommost region of each melt pool remains unremelted during subsequent passes. The height of this unremelted region approximately corresponds to the prescribed layer thickness (40 μm in the present study), giving rise to the characteristic fish-scale pattern. Under steady-state conditions, the melt pool depth remains approximately constant across layers; consequently, the unremelted height is geometrically equal to the layer thickness. This was confirmed by measurement from specimens, which yielded an unremelted height of approximately 40 μm . This implies that the critical region governing microstructural continuity within each melt pool is the unremelted zone at its base. Accordingly, to quantify the thermal gradient orientation within the bottom 40 μm of the melt pool, the angular distribution relative to the Z-axis is plotted in Fig. 7(a–c), where the insets indicate the relative proportion of the unremelted region with respect to the overall melt pool size. Based on the spatial relationships between adjacent melt pools under each condition, the regions at the melt pool bottom that are remelted by adjacent melt pools (indicated in blue) and upper melt pools (indicated in yellow) are delineated accordingly.

In cubic crystal systems, the preferred rapid growth direction $\langle 100 \rangle$ tends to align with the local thermal gradient. Under the 150 W condition, the shallower melt pool results in a larger fraction occupied by the unremelted zone, leading to a wider angular spread of thermal gradient orientations within this region; the maximum angle relative to the Z-axis is calculated to be approximately 60° . This broader angular span makes

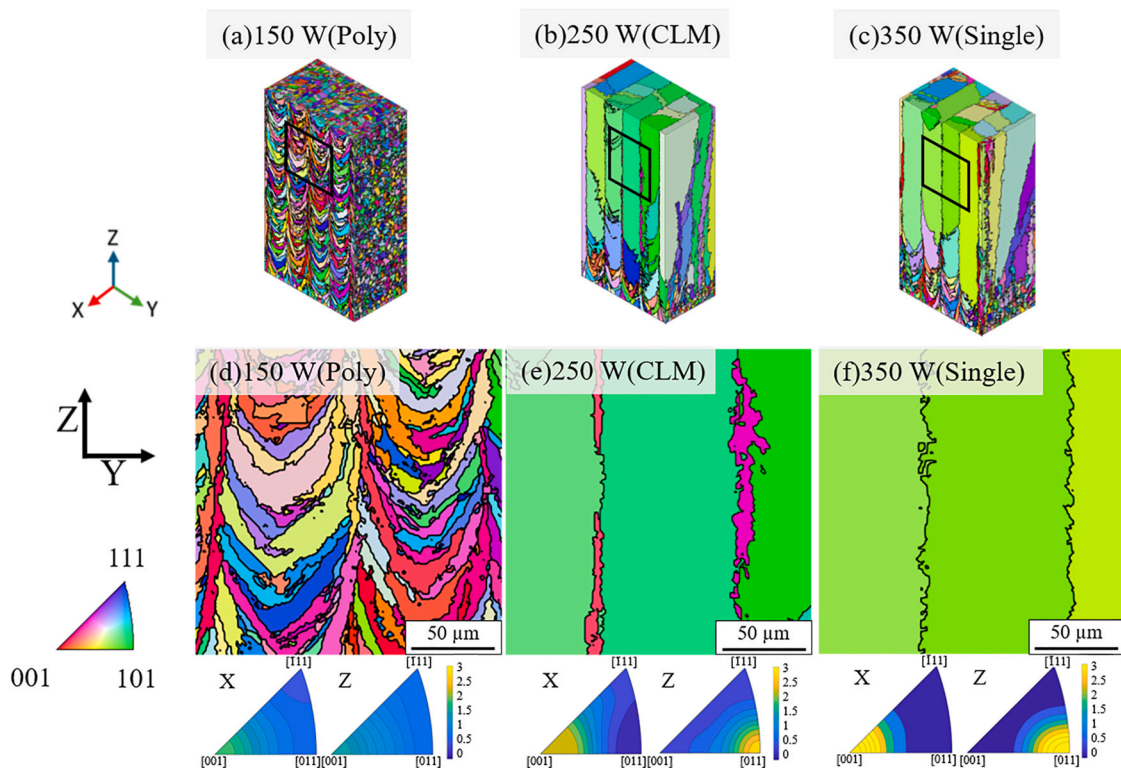


Fig. 5. (a–c) Microstructures simulated using ExaCA under different laser power conditions. (d–f) Cross-sectional IPF maps along the build direction extracted from the simulations.

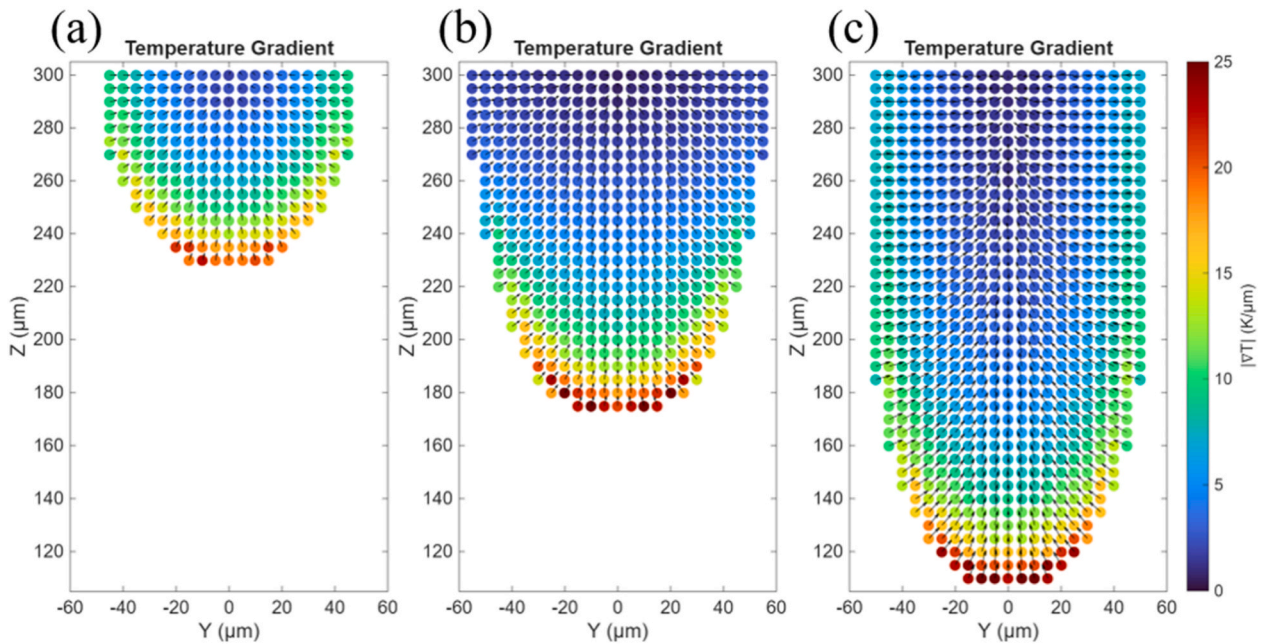


Fig. 6. Cross-sectional thermal gradient distributions of the melt pool under different laser power conditions: (a) 150 W, (b) 250 W, and (c) 350 W.

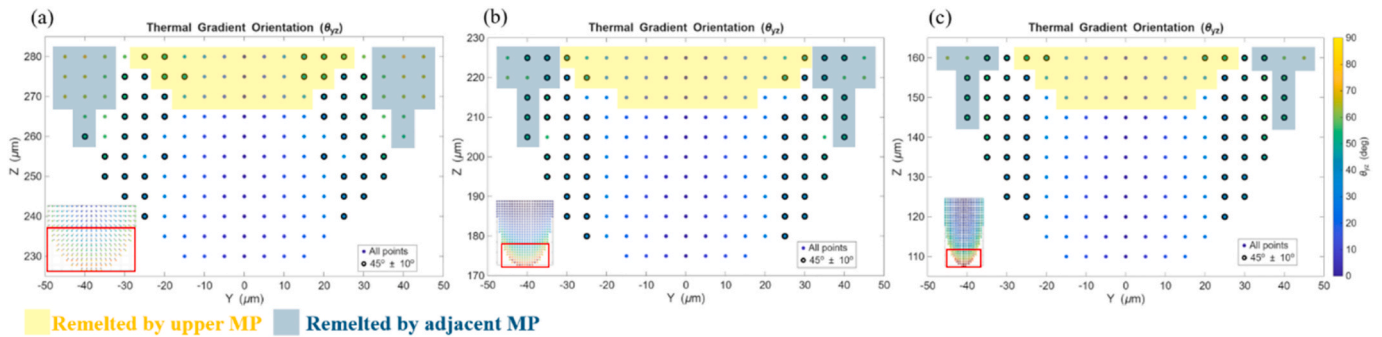


Fig. 7. Distributions of the thermal gradient angle relative to the Z-axis at the bottom of the melt pool at (a) 150 W, (b) 250 W, and (c) 350 W. The insets illustrate the unremelted region relative to the total melt pool area.

it difficult for dendrites to maintain a consistent growth orientation across the unremelted zone, thereby hindering epitaxial continuity. Furthermore, virtually no nodes with a 45° angle are present at the intersection with adjacent melt pools, and the thermal gradient directions of adjacent melt pools subtend an angle exceeding 90° , so a single dendrite growth direction cannot remain favorably aligned with

the thermal gradients on both sides. This misalignment disrupts coherent epitaxial growth across neighboring tracks. In contrast, for the 250 W and 350 W conditions, the angular span of the thermal gradient in the unremelted zone is comparatively narrower, with a maximum angle of approximately 45° . Both conditions exhibit a notable concentration of nodes at approximately 45° in the overlap regions, implying that the

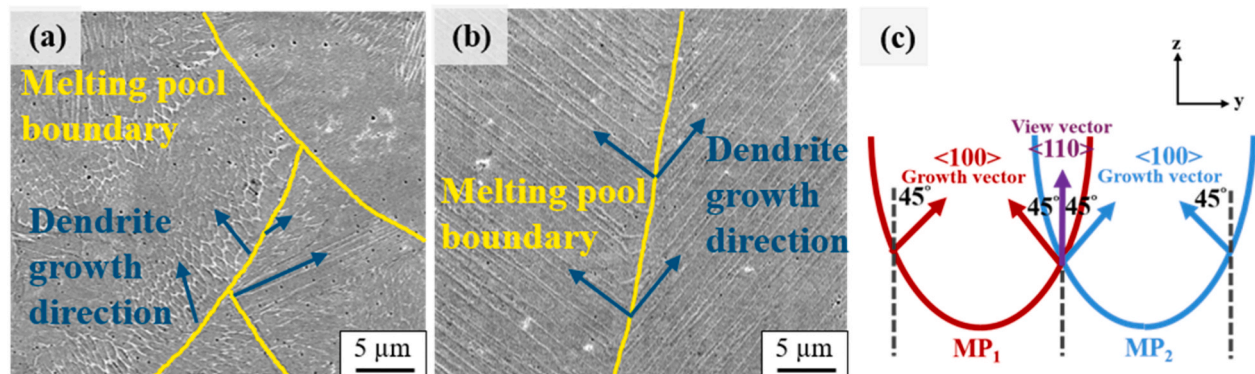


Fig. 8. SEM micrographs highlighting melt pool boundaries and preferred dendrite growth directions for (a) 150 W and (b) 250 W samples (representative of 350 W). (c) Schematic illustration of the dendrite growth competition and orientation relationship between adjacent melt pools during the formation of the major layer.

dendrite growth directions in adjacent melt pools are mutually perpendicular. This geometric relationship enables pre-existing dendrites to continue epitaxial growth in a coherent and continuous manner, which accounts for the large, contiguous grains oriented along the $\langle 110 \rangle$ direction observed in the EBSD maps.

The corresponding SEM micrographs of dendrite growth orientations and a schematic illustration of dendrite growth competition and orientation relationships are presented in Fig. 8. Fig. 8(a), taken from the 150 W condition, reveals that the dendrite growth directions within the melt pool are relatively disordered and that the dendrite arrangements between adjacent melt pools also lack regularity. In contrast, Fig. 8(b), obtained from the 250 W condition (with the 350 W condition exhibiting an identical trend), demonstrates that the dendrites within a single melt pool are uniformly aligned along the same direction and that the dendrites in adjacent melt pools are oriented perpendicular to each other. This mechanism is further illustrated schematically in Fig. 8(c). At the melt pool bottom, the thermal gradient is oriented at approximately 45° to the Z-axis, and dendrites grow along the $\langle 100 \rangle$ growth vector that best aligns with this local gradient. Upon remelting by an adjacent track, the thermal gradient in the overlap region is mirrored to the opposite 45° orientation, prompting epitaxial regrowth along another $\langle 100 \rangle$ growth vector perpendicular to the original one. Because these two mutually perpendicular $\langle 100 \rangle$ growth vectors are each inclined at 45° to the Z-axis, their resultant crystallographic orientation projected onto the build direction corresponds to the $\langle 110 \rangle$ view vector. This continuous epitaxial growth across neighboring melt pools ultimately gives rise to the macroscopic $\langle 110 \rangle // Z$ texture observed in the major layer. These observations constitute a direct, spatially resolved measurement of the gradient orientation that prevailed during solidification, and therefore provide an experimental check on the simulated gradient field that is independent of the melt pool dimensions compared in Section 3.1. The distinction is important: agreement in melt pool geometry constrains the energy deposition and the shape of the liquidus isotherm, whereas the dendrite orientations constrain the direction of the thermal gradient, which is the quantity on which the present mechanism depends.

To quantitatively evaluate the evolution of the crystallographic texture with deposited layers, the texture quantification metric, M-index, was measured along the build direction. The M-index is defined as [56]:

$$M = \frac{1}{2} \int |f_{MDF}^U(\theta) - f_{MDF}(\theta)| d\theta \quad (13)$$

where f_{MDF}^U denotes the uncorrelated misorientation distribution function (MDF) of a random uniform distribution, and f_{MDF} is the obtained MDF from EBSD data. The M-index ranges from 0 (random texture) to 1 (single crystal) and was calculated for each XY slice along the build direction, excluding the layer affected by the final laser scan, which has not been remelted and is therefore not representative of the steady-state microstructure. The results are presented in Fig. 9. Under all three conditions, the initial state corresponds to a randomly oriented powder layer. Under the 150 W condition, the M-index remains at a consistently low level regardless of increasing build height, indicating that the texture remains nearly random throughout the build. In contrast, under the 250 W and 350 W conditions, the M-index progressively increases with build height, reflecting a competitive grain selection process in which grains capable of maintaining epitaxial growth under the local thermal-gradient configuration near the melt pool bottom are preferentially retained, ultimately giving rise to the dominant major $\langle 110 \rangle // Z$ layer.

4.2. Competitive growth of minor $\langle 100 \rangle // Z$ layer

To clarify the origin of the minor $\langle 100 \rangle // Z$ layer that appears only in the 250 W condition, the simulation-derived thermal gradient was further decomposed into its Y and Z components. This analysis reveals that the minor layer is governed by the local balance between the lateral (Y) and vertical (Z) components of the thermal gradient near the melt pool bottom, as shown in Fig. 10. From Fig. 10(a and b), it can be observed that under both conditions, the Y-component of thermal gradient is distributed along the lateral sides of the melt pool, with a low-gradient region in the center, whereas the Z-component is concentrated at the bottom of the melt pool and exhibits a higher magnitude. Such a gradient distribution gives rise to a central region where the thermal gradient is predominantly aligned with the Z-axis, favoring the epitaxial growth of $\langle 100 \rangle$ -oriented dendrites along the build direction and thereby promoting the formation of the minor layer. Furthermore, to elucidate why the formation of the minor layer is suppressed under the 350 W condition, the Y-component of the thermal gradient under both conditions was magnified, and a threshold value was applied to identify the nodes where the thermal gradient direction is nearly aligned with the build direction, as shown in Fig. 10(c and d). Given that the Z-component at the melt pool bottom was approximately $25 \text{ K}/\mu\text{m}$ across all conditions, a threshold of $|dT/dy| < 7 \text{ K}/\mu\text{m}$ was adopted to identify regions of low lateral thermal gradient. This value corresponds to

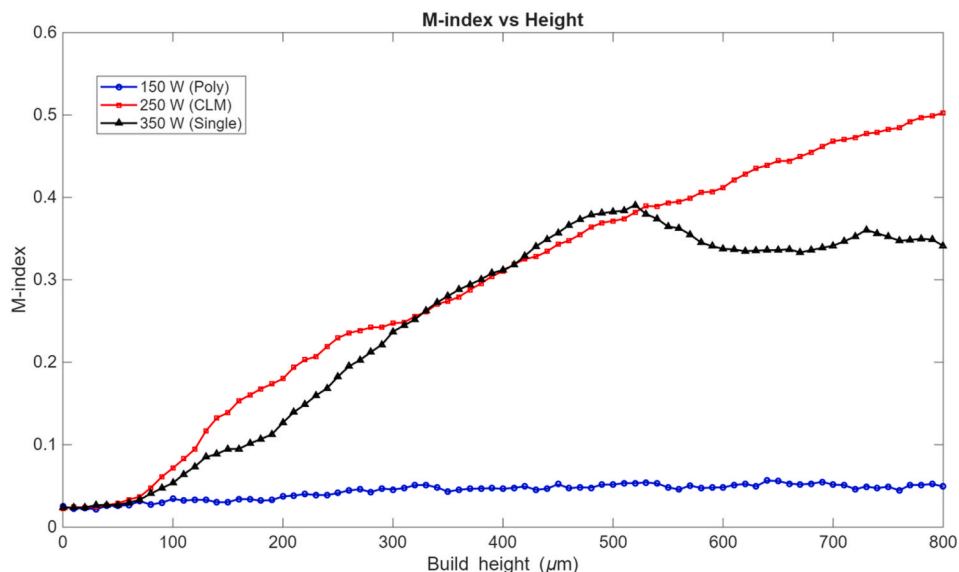


Fig. 9. Evolution of the M-index along the build height.

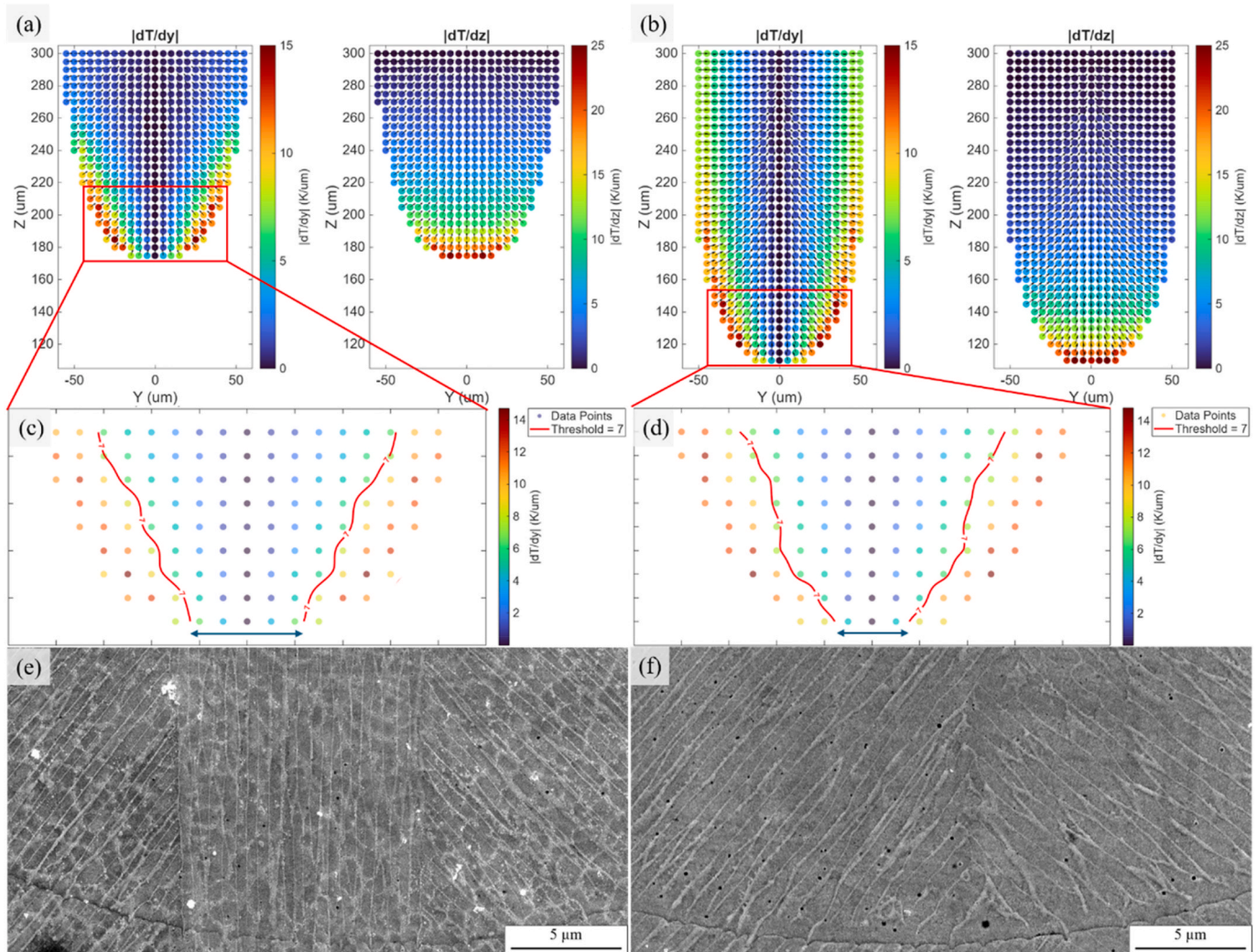


Fig. 10. Decomposition of thermal gradients and correlation with melt pool bottom microstructures: (a, c, e) 250 W and (b, d, f) 350 W. Panels (a–b) show the Y- and Z-direction components of the thermal gradient; (c–d) present magnified views of the Y-direction gradient with a threshold value of 7 indicated; and (e–f) show SEM images of the melt pool bottom.

approximately 15° from the build direction where $|dT/dz|$ attains its maximum at the deepest part of the melt pool. Such regions are favorable for the epitaxial growth of $\langle 100 \rangle$ -oriented dendrites along the build direction. By comparison, the 250 W condition exhibits a wider low-Y-gradient region, which allows $\langle 100 \rangle$ -oriented dendrites to undergo epitaxial growth without being disrupted by lateral thermal gradients. In contrast, under the 350 W condition, the melt pool transitions into keyhole mode, resulting in a narrower and deeper melt pool geometry. This elongated morphology renders the Y-component of the thermal gradient more pronounced, thereby narrowing the low-Y-gradient region and inhibiting the epitaxial growth of $\langle 100 \rangle$ -oriented dendrites. Consequently, the formation of the minor layer is suppressed under the 350 W condition, whereas it is facilitated at the bottom of the melt pool under the 250 W condition, giving rise to the CLM, as illustrated in Fig. 10(e and f).

4.3. Limitations and scope of the present framework

Although the proposed framework demonstrates its capability in predicting solidification microstructure under various PBF-LB processing conditions, several aspects remain that could be further refined in future studies. First, the thermal history used in the solidification simulation was derived from a single-track thermal model and

subsequently translated to construct the multi-track, multi-layer temperature field. This approach assumes that the thermal conditions remain approximately steady-state across successive tracks and layers. The average effect of inter-layer heat accumulation is represented through the elevated initial temperature, but its progressive evolution is not resolved. A thermal model that resolves this evolution would be a worthwhile extension of the present framework. Second, the latent heat of fusion was not included in the thermal calculation. As shown in [Supplementary Fig. S1](#), including it reduces the magnitude of the thermal gradient, while the orientation of the gradient within the unmelted region at the melt pool bottom is essentially unchanged. According to Eqs. (11) and (12), the gradient orientation is determined by the spatial distribution of the solidification-time field rather than by the magnitude of the thermal gradient. Therefore, although the inclusion of latent heat affects the magnitude of the thermal gradient, its influence on the gradient orientation relevant to the proposed CLM formation mechanism is limited. Third, as stated in Section 2.2.2, the melt pool flow field is not explicitly resolved, and convective heat transport is represented only in an effective manner through the elevated liquid-phase thermal conductivity. Consequently, the model cannot capture flow-induced local variations in the thermal field and solidification front. Explicitly incorporating melt pool flow and convection would be a promising direction for further improving the

physical fidelity of the model. Fourth, the nucleation density in the solidification simulation was set to zero, so that all grain growth occurs epitaxially from previously solidified material. This assumption was examined in two ways. The solidification conditions extracted from the thermal field lie within the fully columnar regime of the columnar-to-equiaxed transition map (Supplementary Fig. S2), and simulations repeated with a finite nucleation density of $N_0 = 1 \times 10^{15} \text{ (m}^{-3}\text{)}$ reproduce the CLM at 250 W and the weakly textured structure at 150 W (Supplementary Fig. S3). This indicates that the CLM is governed by the epitaxial selection mechanism rather than by nucleation behavior, and the weakly textured structure reflects the survival of the initial powder-layer orientations under weak epitaxial selection. Fifth, the framework predicts grain-scale crystallographic orientation selection, that is, which orientations are retained through competitive growth across adjacent tracks and successive layers. It does not resolve the sub-grain cellular substructure, the distribution of solute microsegregation, or intragranular orientation spread, which are governed by solute redistribution on a length scale below that represented by a cellular automaton in which dendritic growth is approximated by an octahedral envelope. These sub-grain features are nevertheless relevant to the mechanical behavior of PBF-LB material and will be addressed in the property assessment that follows this work. Finally, the present framework was developed and validated based on SS316L, an FCC alloy in which the preferred dendrite growth direction is well established along (100). Its extension to alloy systems with different preferential growth directions would require corresponding modifications to the growth kinetics and crystallographic relationships in the model.

5. Conclusion

In this study, a numerical simulation approach was employed to investigate the solidification microstructural evolution of SS316L during the PBF-LB process, with the aim of elucidating the formation mechanism of the CLM. The temperature distribution within the melt pool under different laser conditions was first obtained through FEM thermal simulations and subsequently imported into ExaCA to simulate the resulting microstructure. The main findings are summarized as follows:

1. The adopted heat source model accurately captured the melt pool dimensions under various processing conditions. Combined with ExaCA simulations, the framework successfully reproduced the experimentally observed microstructural features, demonstrating the reliability of the proposed simulation methodology.
2. A typical CLM, characterized by alternating major $\langle 110 \rangle / Z$ and minor $\langle 100 \rangle / Z$ layers, was reproduced under appropriate processing conditions, indicating that the simulation framework is capable of capturing the essential mechanism of layered texture formation during PBF-LB.
3. The formation of the major $\langle 110 \rangle / Z$ layer is governed by the thermal gradient direction in the overlap region near the bottom of adjacent melt pools. In this region, the local gradient orientation determines whether coherent epitaxial growth can occur across neighboring tracks, while the subsequent competitive grain selection leads to the development of the major layer.
4. The formation of the minor $\langle 100 \rangle / Z$ layer is controlled by the Y and Z components of the thermal gradient near the center of the melt pool bottom. When a sufficiently wide low-Y-gradient region is present, $\langle 100 \rangle$ -oriented dendrites can grow epitaxially along the build direction without being disrupted by lateral thermal gradients, thereby enabling the formation of the minor layer and the resulting CLM.

CRedit authorship contribution statement

Chincheng TSAI: Writing – original draft, Conceptualization, Investigation, Methodology, Software, Validation.; Fabien Briffod: Writing –

review and editing, Conceptualization, Software, Methodology.; Makoto Watanabe: Writing – review and editing, Resources.; Takayuki Shiraiwa: Writing – review and editing, Conceptualization, Resources, Project administration, Supervision, Funding acquisition.

Data availability statement

The data will be made available upon request.

Declaration of generative AI use

During the preparation of this work, the authors used ChatGPT in order to improve the readability and overall language quality of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jmrt.2026.09.255>.

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