Integrated Thermal and Metallurgical Simulation Framework for Selective Laser Melting Multi-Component and Multi-Phase Alloys

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Abstract: To fully understand the impact of cyclic heating on the solid-state phase transformation behavior (SPTB) of multi-component multi-phase alloys (MCPA) during selective laser melting (SLM) and to provide possibilities for the precise customization of the material microstructure, a thermal-metallurgical coupling framework (TMCF) was developed. This framework integrates (1) an equivalent micro-zone heat source model and (2) a Johnson–Mehl–Avrami (JMA) phase transformation kinetic model. Using IN738 superalloy as an example, TMCF was effectively employed to predict the distribution and evolution of the \( \gamma' \) phase during SLM. The results showed that the post-printing distribution of the \( \gamma' \) phase is non-uniform, resulting from the interaction between the precipitation and dissolution behaviors occurring at varying temperatures across distinct spatial locations. Furthermore, the dependence of the \( \gamma' \) phase on the SLM mode was quantitatively estimated. Specifically, the maximum volume fraction of the \( \gamma' \) phase increased by a factor of 17.377, 60.780, and 5.214 when the laser power, scanning speed, and hatch spacing were modified by +50%, −25%, and −16.7%, respectively, within the process window. This finding can provide reference for the fabrication of additional MCPA. In this work, the thermal model within the TMCF was verified by the experimental data reported in the literature.

Keywords: selective laser melting; numerical simulation; thermal metallurgical model; solid-state phase transition

1. Introduction

SLM is an advanced manufacturing technology that has gained significant attention due to its ability to produce complex metal components directly from metal powders, with high precision. This technology exhibits several distinctive features, including a high flexibility in regards to design freedom, minimal tooling requirements, efficient material utilization, and excellent batch consistency, affording it extensive applications in the medical and aerospace industries [1–3]. While the promise of this technology has garnered increasing interest from researchers, who are actively broadening its applications, practical challenges persist. One of the prominent challenges revolves around the limited ability to predict the microstructure and phase composition of materials in the process because most of the printed materials are MCPA, and the SPTB of the material is carried out through the “printing” and “post-processing” stages; moreover, and the level of regulation directly affects the performance of the part [4–6]. Indeed, the complex manufacturing strategies, coupled with the dynamics of layer-by-layer printing, subject the material to complex temperature history, constituting a primary limiting factor for accurately predicting microstructural conditions [7–9]. Moreover, for partially precipitation-strengthened materials,
when the additional control of the precipitation phase during the post-processing treatments of the printed part is inappropriate, strain age cracking (SAC) may be induced, directly leading to macro-scale cracking. Therefore, investigating the microstructure and phase transformation mechanisms in components undergoing complex thermal cycling can help to fully exploit this technology’s potential, including the provision of new ideas to avoid SAC and the achievement of precise customization of the structure.

Presently, researchers primarily establish the relationship between process parameters and material characteristics in SLM through “experiment and characterization” and “computational modeling” [10,11]. The “experiment and characterization” method primarily involves the post-printing assessment of the component microstructures at room temperature to deduce the material–process–structure relationship [12,13]. For example, Bergmueller et al. [13] introduced a high-powered speckle laser beam for in situ heat treatment during the SLM preparation of PM HS 10-2-5-8 high-speed steel, which enabled them to develop a novel approach for achieving fine equiaxed grain microstructures. However, this method is associated with a time lag, making it challenging to clarify the evolving process and the formation mechanisms of critical information during the process, making it difficult to form a standard solution suitable for diverse materials. Furthermore, a few researchers obtain process information through in situ detection methods, encompassing data related to the evolution kinetics of the molten pool [14,15] and the phase transition behavior [16,17]. These detection methods primarily include in situ X-ray imaging and X-ray scattering techniques. For example, Wahlmann et al. [16] investigated the $\gamma/\gamma'$ phase transformation during the SLM process of CMSX-4 nickel-based superalloy using X-ray scattering, which helps to describe the phase composition change of the material during the printing process. However, this method has not been widely used due to the limitations regarding experimental space–time resolution, experimental error control levels, experimental costs, and other factors.

In contrast, using computational modeling techniques to study SLM is considered low-cost and promising, and it helps to identify the microstructure evolution from multiple scales and to achieve related attribute prediction [18–20]. At present, there are two main applications of this technique. One is to study the complex physical phenomena, such as heat transfer, solid–liquid conversion, flow, and heat in the mesoscopic metal molten pool area during SLM and to provide a reference for clarifying the mechanism of the formation of defects [21,22]. For example, Wang et al. [22] developed a thermal fluid model that considers physical phenomena such as liquid flow, metal evaporation, and the Marangoni effect, and with the help of the model, the mechanism of pore formation in the additive manufacturing process was discovered, providing insights into preventing pore formation. The other application is to simulate the evolution of microstructure by employing commonly used techniques, including the Monte Carlo, cellular automata, phase field, and other methods. When predicting the material microstructure, it is essential to input temperature data that closely resembles real-world data. Through these methods, successful simulations of both microstructure (i.e., grain characteristics, such as morphology size) and defects (porosity) have been achieved. For instance, Sunny et al. [23] employed the dynamic kinetic Monte Carlo method and successfully predicted the SLM In625 grain structure. However, researchers frequently overlook SPTB within the grains or at the grain boundaries when calculating microstructures [24,25]. The primary reason for neglecting this crucial feature is the difficulty in quantitatively describing the complex phase transformation dynamics of the heat-affected zone under rapid heating and cooling. Hence, it is evident that the main challenges in achieving these predictions are (a) the acquisition of the cyclic temperature history of the mesoscopic powder bed during the printing process, (b) establishing a cross-scale temperature mapping mechanism between the mesoscopic powder bed and microstructure, and (c) providing a comprehensive description of the precipitation and re-dissolution kinetics governing material phase transitions under non-isothermal conditions.

The most effective way to address the above challenges involves appropriately simplifying the heat source model and coupling a phenomenological phase transformation
kinetic model to describe the phase transitions. The JMA model is a representative phenomenological phase transformation kinetics model that enables the prediction of phase transformation processes by considering physical mechanisms such as phase nucleation and growth. It has already been successfully applied to the prediction of SPTB in various metal materials [26,27], including superalloys, titanium alloys, and steel. Based on this concept, several researchers have explored the evolution of SPTB in the Directed Energy Deposition (DED) process. For instance, McNamara et al. [26] employed a non-isothermal JMA model to investigate the precipitation and dissolution behavior of the precipitated phases at specific locations in the DED Ti-6Al-4V process. Furthermore, Adomako et al. [27] coupled a semi-analytical heat source model with MatCalc thermodynamic simulation software to quantitatively describe the phase transition process of the $\gamma'$ phase in the DED IN738 superalloy process. These models successfully capture the SPTB at specific locations across both time and space, providing a reference for an in-depth understanding of the SPTB in DED processes. However, there is limited research on the SPTB of SLM, particularly concerning the evolution of precipitated phases between the components’ basic units (layer-to-layer or track-to-track) during the printing process and its relationship with the process parameters. This restricts the capability to predict the structure and phase composition of the metal components in SLM.

Based on this background, the originality and novelty of this work lie in the combination of appropriate thermal and metallurgical models and the use of the original coupling algorithms to establish a TMCF. This framework can efficiently calculate the phase transformation of the materials within the entire powder bed under multiple thermal cyclings during SLM. Specifically, the thermal model uses an equivalent micro-region heat source model that quantifies the unsteady temperature field evolution of the powder bed from the mesoscopic scale, while the metallurgical model uses a non-isothermal JMA model. Subsequently, using IN738 nickel-based superalloy as a material system, the temperature evolution and the SPTB of the material in the ten-layer and five-track SLM process were studied. Ultimately, an analysis was conducted to evaluate the influence of laser power, scanning speed, and hatch spacing parameters on the evolution of the $\gamma'$ phase. The TMCF presented in this paper holds the potential to enable the precise control of the microstructures.

2. Theoretical Model

The theoretical model mainly consists of both a thermal model and a metallurgical model, in which the thermal model is used to solve the temperature distribution of the three-dimensional unsteady heat transfer process within the powder bed and the component during SLM. In contrast, the metallurgical model mainly describes the phase transition of the MCPA at different times through the non-isothermal JMA model. The following section provides an overview of the assumptions, governing equations, and prescribed boundary conditions pertinent to the formulation of this theoretical model. These considerations were tailored to the unique characteristics of the SLM process. The theoretical model can be solved through the TMCF shown in Figure 1.

2.1. Thermal Model

The thermal model mainly solves the three-dimensional transient heat transfer equation, as expressed in Equation (1) [18], to accurately quantify the temperature evolution throughout the SLM process. As depicted in Figure 1, a crucial aspect of solving this equation lies in the meticulous description of the boundary conditions and initial conditions that dictate temperature variations within the computational domain. These boundary conditions primarily detail the heat input and dissipation behaviors pertinent to the defined region.

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) + Q$$  \hspace{1cm} (1)
where $T$ is temperature, °C; $\rho$ is the density of the metal material, kg·m$^{-3}$; $C_p$ is the specific heat of metal materials, J·kg$^{-1}$·°C$^{-1}$; $k_{xx}$, $k_{yy}$, and $k_{zz}$ are the thermal conductivity of the material along the x, y, and z directions, W·m$^{-1}$·°C$^{-1}$, respectively, with an assumption of isotropy; and $Q$ is the endogenous heat source per unit volume, W·m$^{-3}$.

**Figure 1.** Schematic diagram of the thermal–metallurgical model for SPTB prediction.

### 2.1.1. Heat Input

During the SLM process, heat is predominantly delivered to the upper surface of the powder bed via a high-energy laser. This paper adopts an equivalent micro-zone heat source model to characterize the heat input behavior, as indicated in Equation (2). The development of this heat source model draws heavily from the research findings of Chiumenti et al. [21]. Chiumenti observed that by employing the equivalent micro-zone heat source model to simulate temperature field changes during SLM, especially when the selected micro-zone heat source is significantly smaller in scale than the entire computational domain, the model can aptly capture the evolution of the temperature field. Remarkably, this approach consumes only 1/6 of the computational resources required by the conventional high-fidelity temperature models.

$$Q_{in} = \frac{\eta P}{V_{pool}L} = \frac{\eta P}{v_{Laser}\Delta H-HatchL_{Thick}}$$

(2)

where $\eta$ is the energy efficiency, representing the percentage of laser energy converted to material energy. This parameter exhibits associations with various factors, including powder density, material vapor pressure, and the enthalpy of material phase changes. $P$ is laser power, W; and $V_{pool}$ represents the volume of the metal molten pool under the action of a high-energy laser, which can be calculated by laser scanning speed, time interval, hatch spacing, and layer thickness, m$^3$.

When employing this model, several key assumptions are made. Firstly, it is assumed that the high-energy laser serves as a volumetric heat source acting on the powder bed. As the material temperature exceeds the melting point, the physical parameters transition from the powder phase to that of the bulk material. Secondly, it is assumed that the heat input from the high-energy laser is contingent on variables such as laser power, layer thickness, and the volume of the metal pool. Finally, it is assumed that the thermophysical parameters of the metal materials in the model are temperature and state-dependent, and the transition of these parameters between the metal powder and the bulk material adheres to the relationships delineated in Table 1.
Table 1. Relationship of thermophysical parameters between the powder and bulk materials.

<table>
<thead>
<tr>
<th>Bulk Property</th>
<th>Powder Property Expression</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_{bulk}$</td>
<td>$p_p = p_{bulk}(1 - \varphi) + p_{gas}\varphi$</td>
<td>[20]</td>
</tr>
<tr>
<td>$k_{bulk}$</td>
<td>$k_p = k_f\left(Term_1 + k_f\sqrt{1 - \varphi}Term_2\right)$</td>
<td>[19]</td>
</tr>
<tr>
<td>$\rho_{bulk}$</td>
<td>$\rho_p = \rho_{bulk}\frac{C_{p,\rho_{\text{bulk}}} + \rho_{\text{gas}}\left(1 - \varphi\right)}{C_{p,\rho_{\text{bulk}}}\left(1 - \varphi\right)}$</td>
<td>[20]</td>
</tr>
</tbody>
</table>

2.1.2. Heat Dissipation

In characterizing heat dissipation during the SLM process, it is postulated that the primary modes of heat dissipation for the top layer are thermal convection and thermal radiation, and these play a significant role in dissipating heat from the components during the printing process. Conversely, the heat exchange between the side of the component and the adjacent powder layer is approximated through thermal convection, and the heat dissipation can be expressed as shown in Equation (3). By combining Equation (2) and Equation (3), when the equivalent micro-zone heat source is applied to the component’s surface area, the total heat comprises the sum of the heat input and heat dissipation. The corresponding boundary conditions are provided in Equation (5).

\[
Q_{out} = \left\{ \begin{array}{l}
-h_c(T - T_{amb})|_{\Gamma} \quad \Gamma \in \Lambda_{other} \\
-h_c(T - T_{amb}) - \sigma \epsilon(T^4 - T_{amb}^4)|_{\Gamma} \quad \Gamma \in \Lambda_{top}
\end{array} \right.
\]  

where $h_c$ is the convective heat transfer coefficient, W·m$^{-2}$·K; $T_{amb}$ is the ambient temperature, °C; $\Gamma$ is the surface area of the component; $\Lambda_{other}$ is the side area of the component; $\Lambda_{top}$ is the upper surface area at a certain moment in the component printing process; and $\sigma$ is the Stefan-Boltzmann constant with a value of $5.6704 \times 10^{-8}$ W·m$^{-2}$·K$^4$, along with the emissivity parameter, as described in Equation (4) [19].

\[
\epsilon = \epsilon_{bulk} - 0.908\epsilon_{bulk}\varphi^2 - 1.908\varphi^2 - 2\varphi + 1 - 2 + 3.082\varphi^{-1}(1 - \varphi)^2 \epsilon_{bulk}\left[1 + 3.082\varphi^{-1}(1 - \varphi)^2 \right] + 1
\]  

\[
K(\Delta T \cdot n)|_{\Gamma} = \left\{ \begin{array}{l}
Q_{out}|_{\Gamma} \quad \Gamma \notin \Lambda \\
Q_{in} + Q_{out}|_{\Gamma} \quad \Gamma \in \Lambda
\end{array} \right.
\]  

where $\Lambda$ represents the action area of the laser at a specific moment; $n$ represents the normal direction of the workpiece surface.

2.1.3. Initial Conditions

In the SLM process, initially, the temperature of both the powder bed and the substrate is the ambient temperature, as shown in Equation (6), where $D$ represents the entire computational domain. When the substrate is preheated, the initial temperature within the computational domain of substrate is set to the preheating temperature, while the component’s initial temperature remains at the ambient temperature.

\[
T(x, y, z, 0) |_{t=0} = T_{amb}(x, y, z) \in D
\]

2.2. Metallurgical Model

The metallurgical model primarily encompasses the depiction of SPTB in MCPA, employing the non-isothermal JMA model. As shown in Figure 1, the key input data for this model is the thermal cycling by the material throughout the SLM process. The key element of the model is its capacity to employ the phase transformation evolution model to
describe the precipitation and re-dissolution processes of the material. Considering that the re-dissolution process of the precipitated phase in the material is approximately inversely equivalent to the precipitation and growth process of the matrix phase, this section will center on elucidating the principles behind the non-isothermal JMA model and describing the method for computing the phase transformation kinetics during the precipitation and growth of the precipitated phases, as tailored to the characteristics of the SLM process.

2.2.1. Principles of the JMA Model

Before introducing the non-isothermal JMA theory, several key assumptions are established, considering the unique characteristics of the SLM process:

- It is assumed that within the SLM process, the material’s phase transition under thermal cycling is characterized as a diffusion phase transition, and its phase transition kinetics are related to physical mechanisms, such as nucleation and growth, at the level of the atomic lattice of the substances;
- It is assumed that the SPTB of the material during the printing process can be superimposed by the precipitation behavior of the isothermal section, in which the isothermal section is obtained by dispersing the temperature history over time;
- It is assumed that the phase transition occurring in the isothermal section is contingent upon the degree of reaction and the equilibrium phase fraction.

The solution of the non-isothermal JMA model is presented in Figure 2. It is evident from the figure that for complex non-isothermal processes, especially when the chosen time intervals are sufficiently small, the temperature evolution can be discretized into the summation of a series of isothermal sections. Subsequently, the phase transition in the non-isothermal process can be ascertained by summing the phase variables from multiple isothermal sections. In this way, the evolution of the phase volume fraction with respect to time can be indirectly deduced.

![Figure 2](image-url)
Taking the IN738 superalloy as an example, the fundamental principles of the non-isothermal JMA model is further described, as shown in Equation (7). The IN738 superalloy is a precipitation-strengthened nickel-based superalloy primarily composed of a γ matrix phase and a γ' precipitated phase. There is a transformation between the γ matrix and the γ' precipitated phase in the printing process of the alloy, and the volume fraction of the γ' phase at room temperature exceeds 50%. Combined with Figure 2 and Equation (7), the γ' phase in the SLM process grows and redissolves many times during the reheating process. This precipitation and re-dissolution behavior is chiefly dictated by the relative size of the volume fraction of the γ' phase in the material and the equilibrium volume fraction of the γ' phase at a given temperature. For instance, when the temperature is $T_i$, if the volume fraction of the γ' phase is less than the equilibrium volume fraction of the γ' phase, the γ' phase will continue to precipitate. Consequently, the variation in the volume fraction of the γ' phase is the increment of the precipitated phase within the time interval $\Delta t$ at temperature $T_i$.

\[
\begin{align*}
 f &= \begin{cases} 
 f_{\gamma', \text{grow}}^{\text{ini}} + \sum_{i=1}^{n} f_{\gamma', \text{grow}, \Delta t}^{T_i} & f < f_{\gamma', \text{eq}}^{T_i} \\
 f_{\gamma', \text{eq}}^{T_i} & f = f_{\gamma', \text{eq}}^{T_i} \\
 f_{\gamma', \text{diss}}^{\text{ini}} + \sum_{i=1}^{n} f_{\gamma', \text{diss}, \Delta t}^{T_i} & f > f_{\gamma', \text{eq}}^{T_i}
\end{cases}
\tag{7}
\end{align*}
\]

where $f_{\gamma', \text{eq}}^{T_i}$ is the equilibrium volume fraction of the γ' precipitated phase when the temperature is $T_i$; $f_{\gamma', \text{grow}}^{\text{ini}}$ is the initial volume fraction when the γ' precipitated phase begins to grow; $f_{\gamma', \text{grow}, \Delta t}^{T_i}$ is the precipitation amount of the volume fraction of the γ' precipitated phase within the time interval $\Delta t$ at temperature $T_i$; $f_{\gamma', \text{diss}}^{\text{ini}}$ represents the initial volume fraction when the γ' precipitated phase begins to dissolve; and $f_{\gamma', \text{diss}, \Delta t}^{T_i}$ represents the amount of re-dissolution of the volume fraction of the γ' precipitated phase within the time interval $\Delta t$ at the temperature $T_i$.

2.2.2. Kinetic Calculation of JMA Model

Describing the phase transformation during the precipitation process is achievable by calculating the increment in the γ' phase precipitation within each isothermal period. This computation of the increment in the γ' phase during each isothermal period encompasses three fundamental components: the determination of the equivalent time, the calculation of the reaction degree increment, and the assessment of the increment in the volume fraction of the γ' phase. To facilitate the quantitative analysis of the precipitation process, the following assumptions are established:

- It is assumed that within the $t_i$-$t_{i+n}$ time interval, the γ' phase in the IN738 superalloy continues to precipitate and grow. At the outset, the volume fraction of the γ' phase at $t_i$ is $f_{\gamma', \text{grow}}^{\text{ini}}$, and the total time is divided into $n$ parts;
- It is assumed that the time interval $\Delta t$ and the temperature interval $\Delta T_i$ are both sufficiently small positive values, and the material’s temperature remains constant within each period, in which the interval time $t_i$-$t_{i+1}$ corresponds to the temperature $T_i$, while the interval time $t_{i+1}$-$t_{i+2}$ corresponds to the temperature $T_{i+1}$, etc.

During the time interval $t_i$-$t_{i+1}$, the equivalent time means that the initial γ' phase fraction $f_{\gamma', \text{grow}}^{\text{ini}}$ is transformed into the time $t_{\xi_i}$, completely corresponding to the precipitation of temperature $T_i$, and the derivation process of $t_{\xi_i}$ is shown in Equations (8)–(10).

\[
\xi_{T_i} = 1 - \exp\left(-k(T_i)I_{ss}^{n}\right) \tag{8}
\]

where $n$ is the Avrami index, taking 2.5; $k(T_i)$ is the reaction rate constant, expressed as $k(T) = \frac{8\mu}{15}I_{ss}^{3/2}$, where $I_{ss}$ is used to describe nucleation, expressed as $I_{ss} = \ldots$
ZN_0 \gamma^* \exp(-\Delta G^{*}k_B^{-1}T^{-1})$, and $\mu$ is used to describe diffusion growth, expressed as

$$\mu = \sqrt{2D \left( c_0 - c_0^eq \right) \left( c_\gamma^eq - c_\gamma^eq \right)^{-1}}.$$  

where $f_{\gamma^*_\text{grow}}^{ini}$ represents the equilibrium volume fraction of the $\gamma'$ phase at temperature $T_i$.

$$f_{\gamma^*_\text{grow}}^{ini} = \xi_{T_i} \cdot \left( f_{\gamma^*_\text{eq}}^{ini} - f_{\gamma^*_\text{grow}}^{ini} \right)$$  

The reaction degree increment refers to the increment of the reaction degree of the $\gamma'$ phase after time $t_{gi}$, based on the equivalent precipitation time $\Delta t$. The derivation is shown in Equations (11) and (12).

$$\xi_{T_i,t_{gi}+\Delta t} = 1 - \exp \left( -k(T_i)(\Delta t + t_{gi})^n \right)$$  

where $\xi_{T_i,t_{gi}+\Delta t}$ represents the reaction degree of the $\gamma'$ phase at temperature $T_i$ when the equivalent time is $t_{gi} + \Delta t$.

$$\xi_{T_i,t_{gi}+\Delta t} = \xi_{T_i,t_{gi}+\Delta t} - \xi_{T_i,t_{gi}}$$  

The increment of the $\gamma'$ phase volume fraction refers to the increment of the $\gamma'$ phase during the time interval $\Delta t$ at temperature $T_i$, which can be obtained by the product of the increment of the reaction degree in Equation (12) and the potential difference of the volume fraction of the precipitated phase, as shown in Equation (13).

$$f_{\gamma^*_\text{grow},\Delta t}^{T_i} = \xi_{T_i,\Delta t} \cdot \left( f_{\gamma^*_\text{eq}}^{ini} - f_{\gamma^*_\text{grow}}^{ini} \right)$$  

For the time interval $i_{i+1} - t_{i+2}$, the initial volume fraction of the $\gamma'$ phase is the sum of $f_{\gamma^*_\text{grow}}^{ini}$ and $f_{\gamma^*_\text{grow},\Delta t}$, as shown in Equation (14). Equations (14) and (15) can be updated to obtain the volume fraction of the $\gamma'$ phase at time $t_{i+1}$ and temperature $T_{i+1}$. At this time, the increment of the $\gamma'$ phase volume fraction during $t_{i+1} - t_{i+2}$ can be obtained by combining Equations (10)–(13).

$$f_{\gamma^*_\text{grow}}^{ini} = f_{\gamma^*_\text{grow}}^{ini} + f_{\gamma^*_\text{grow},\Delta t}^{T_i}$$  

$$i = i + 1$$  

Based on this method, the volume fraction increment of the $\gamma'$ phase in any sub-interval within the time interval $t_i - t_{i+n}$ and the volume fraction of the $\gamma'$ phase at any time can be obtained by sequential iteration.

### 3. Numerical Model

Based on the finite element technology, the TMCF is established in a “strong coupling” manner, as shown in Figure 1. This framework, in conjunction with the pertinent material parameters and boundary conditions within the SLM environment, is employed to portray the evolution of both the temperature field and the precipitated phase fraction during the SLM process. The “strong coupling” signifies that the temperature distribution and the phase composition calculations occur in each incremental step. The specific details pertaining to the numerical simulation model are outlined as follows.
3.1. TMCF Modeling

Before establishing the TMCF, the following assumptions are made to balance the relationship between the accuracy and calculation time and to accurately and efficiently describe the process’s temperature field and phase composition.

- It is assumed that the layer-by-layer printing in the actual process can be described using the “birth and death method” to activate the dead unit layer by layer, wherein the thickness of the powder layer of the model is the same as that of the actual physical layer;
- The JMA model is mainly used to describe the phase change behavior at the microscopic scale (µm), and the computational domain in this work is the powder bed at the mesoscopic scale (mm). There are scale differences when applying this model, so it is assumed that the node’s phase fraction in the powder bed model (the horizontal distance between nodes is 50 µm) can represent the average phase fraction within the node’s neighboring microregions;
- Considering the slow diffusion-type phase transformation reaction rate at low temperatures, only the phase transformation behavior of the IN738 superalloy at temperatures above 600 °C is considered.

Based on the above assumptions, TMCF was established using Abaqus 2018 software.

3.2. Simulation Parameters

The simulation parameters primarily include the material parameters and boundary conditions, where the material parameters consist of the composition, the thermal physical parameters, and the phase transformation kinetic parameters of the IN738 superalloy, as detailed in Tables 2 and 3 and Figure 3, respectively. The thermal conductivity, specific heat, and density of the IN738 superalloy bulk materials are given in Table 3, and the properties of the corresponding powder materials can be calculated in combination with the equations listed in Table 1. Figure 3 shows the parameters characterizing the equilibrium phase fractions, precipitation, and re-dissolution behavior of the IN738 superalloy. The precipitation parameters include the isothermal transformation curves and the kinetic parameter describing γ' phase nucleation and growth, as depicted in Figure 3b,c. On the other hand, the re-dissolution parameters include the gamma phase interface position and the gamma interface growth rate, as shown in Figure 3d,f. These parameters are predominantly computed using the Thermo-Calc 2023a, JmatPro 12.1 software and Equation (8).

Table 2. Composition of the IN738 superalloy (wt.%) [28].

<table>
<thead>
<tr>
<th>Element</th>
<th>C</th>
<th>Si</th>
<th>Cr</th>
<th>Co</th>
<th>Mo</th>
<th>W</th>
<th>Nb</th>
<th>Ta</th>
<th>Al</th>
<th>B</th>
<th>Ni</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wt%</td>
<td>0.11</td>
<td>0.02</td>
<td>15.85</td>
<td>8.37</td>
<td>1.8</td>
<td>2.66</td>
<td>0.89</td>
<td>3.39</td>
<td>1.8</td>
<td>3.38</td>
<td>0.007 Bal.</td>
</tr>
</tbody>
</table>
Table 3. Thermal properties of the IN738 superalloy used in TMCF [28,29].

<table>
<thead>
<tr>
<th>T [°C]</th>
<th>( K_{\text{bulk}} ) [W m(^{-1}) K(^{-1})]</th>
<th>( C_{p,\text{bulk}} ) [J kg(^{-1}) K(^{-1})]</th>
<th>( \rho_{\text{bulk}} ) [kg m(^{-3})]</th>
<th>( T_{f} ) [°C]</th>
<th>( K_{\text{bulk}} ) [W m(^{-1}) K(^{-1})]</th>
<th>( C_{p,\text{bulk}} ) [J kg(^{-1}) K(^{-1})]</th>
<th>( \rho_{\text{bulk}} ) [kg m(^{-3})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>8.55</td>
<td>414.7</td>
<td>8190</td>
<td>800</td>
<td>21.75</td>
<td>658.7</td>
<td>7900</td>
</tr>
<tr>
<td>200</td>
<td>11.57</td>
<td>468.8</td>
<td>8130</td>
<td>1000</td>
<td>25.14</td>
<td>717.6</td>
<td>7790</td>
</tr>
<tr>
<td>400</td>
<td>14.96</td>
<td>529.0</td>
<td>8060</td>
<td>1200</td>
<td>28.54</td>
<td>782.5</td>
<td>7650</td>
</tr>
<tr>
<td>600</td>
<td>18.36</td>
<td>589.2</td>
<td>7990</td>
<td>1400</td>
<td>28.54</td>
<td>855.2</td>
<td>7250</td>
</tr>
</tbody>
</table>

Figure 3. Parameters of the JMA model for the IN738 superalloy. (a) Equilibrium fraction of the \( \gamma^\prime \) phase. (b) Isothermal transformation curve. (c) Kinetic parameter of the \( \gamma^\prime \) phase. (d) \( \gamma-\gamma^\prime \) phase interface position as a function of time. (e) \( \gamma-\gamma^\prime \) phase interface position as a function of the root of time. (f) \( \gamma \) phase parabolic thickening rate.
The information regarding the TMCF and its boundary conditions is shown in Figure 4. The element type is the DC3D8 hexahedral element, which offers higher computational accuracy and faster computational speeds than those of the tetrahedral elements. Furthermore, considering the significant temperature gradient within the area in which the high-energy lasers are loaded during the printing process, mesh subdivision is necessary for the component area and its contact zone; the mesh size is \( 50 \times 50 \times 15 \) µm, while in the remaining regions, the mesh seed density can be appropriately reduced. The boundary conditions of the TMCF encompass both heat input and dissipation. The high-energy laser introduces the heat input through a body heat source in a zigzag scanning pattern, with input values contingent upon the scanning power and scanning speed, among other parameters, as detailed in Section 3.3, and the heat input during the printing process can be calculated using Equation (2). In contrast, heat dissipation is predominantly exhibited by the printed component’s upper surface and sides. On the upper surface, heat dissipates through convection and radiation into the surrounding medium, with convective and radiation heat transfer coefficients set at 10 W·m\(^{-1}\)·°C\(^{-1}\) and 0.3, respectively. Conversely, the heat dissipation from the high-energy laser area to the surrounding powder during the printing process is relatively minimal. An equivalent convective heat transfer coefficient of 5 W·m\(^{-1}\)·°C\(^{-1}\) is employed to facilitate its description through equivalent thermal convection. The coefficients set for the above heat dissipation are empirical values, set within the reference range and in accordance with the characteristics of the equipment, following the methods of references [21,22,30]. As for the substrate, it is essential to consider that the printing process is under a continual state of heat preservation, thus necessitating the lower surface’s engagement in thermal contact heat transfer, with a constant surface temperature of 200 °C. Additionally, combined with the actual printing process, the initial temperatures for the powder, chamber atmosphere, and substrate are 45 °C, 45 °C, and 200 °C, respectively, with a waiting time between the adjacent layers of 8 s during the printing process.

![Figure 4. Mesh and boundary conditions.](image)

### 3.3. Simulation Schemes

To assess the impact of critical process parameters on the behavior of the \( \gamma' \) phase in the IN738 superalloy during the SLM process, seven schemes were designed, as shown in Table 4. The parameters include laser power, scanning speed, and hatch spacing. The energy densities of the laser calculated by these schemes are all in the range of 50–100.0 J·mm\(^{-3}\), and according to the study by Perevoshchikova et al. [31], the energy densities in this range belong to the optimized process window. This is of interest for realistic printing, as shown in Table 4, and the energy density calculation formula is shown in Equation (16).

\[
E = \frac{P}{V_{laser}L_{hatch}L_{thick}}
\]  

(16)
where $E$ represents the energy density of the laser; $P$ represents the laser power; $V_{laser}$ represents the laser scanning speed; $L_{hatch}$ represents the scanning interval; and $L_{thick}$ represents the layer thickness.

**Table 4.** Quantitative scheme showing the influence of the process parameters on the precipitation behavior.

<table>
<thead>
<tr>
<th>Influencing Factor</th>
<th>Case</th>
<th>Laser Power [W]</th>
<th>Laser Speed [mm·s$^{-1}$]</th>
<th>Hatch Spacing [µm]</th>
<th>Layer Thickness [µm]</th>
<th>Laser Energy Density [J·mm$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>R</td>
<td>200</td>
<td>1000</td>
<td>100</td>
<td>30</td>
<td>66.7</td>
</tr>
<tr>
<td>Laser power</td>
<td>A1</td>
<td>250</td>
<td>1000</td>
<td>100</td>
<td>30</td>
<td>83.3</td>
</tr>
<tr>
<td></td>
<td>A2</td>
<td>300</td>
<td>1000</td>
<td>100</td>
<td>30</td>
<td>100.0</td>
</tr>
<tr>
<td>Laser speed</td>
<td>B1</td>
<td>200</td>
<td>750</td>
<td>100</td>
<td>30</td>
<td>88.9</td>
</tr>
<tr>
<td></td>
<td>B2</td>
<td>200</td>
<td>1250</td>
<td>100</td>
<td>30</td>
<td>53.3</td>
</tr>
<tr>
<td>Hatch spacing</td>
<td>C1</td>
<td>200</td>
<td>1000</td>
<td>83</td>
<td>30</td>
<td>80.0</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td>200</td>
<td>1000</td>
<td>125</td>
<td>30</td>
<td>53.3</td>
</tr>
</tbody>
</table>

### 3.4. Thermal Model Verification

The accuracy of the temperature field simulation forms the foundation for quantifying the SPTB. Therefore, in accordance with the experimental work of Chiumenti et al. [21], TC4 material was used to verify the boundary conditions of the thermal model in the TMCF. The validation results are presented in Figure 5. In Figure 5, the experimental data were acquired through a sequence involving “interrupting printing, removing powder, arranging thermocouples, resurfacing powder, and temperature acquisition”. Conversely, the simulation data is obtained by combining the thermal model established in this work with the geometry model and process parameters simulated in the literature. From the comparison of the two types of results, the thermal model can better reflect the temperature change of the components in the actual process, which indicates that the thermal analysis model exhibits a high degree of accuracy and can provide temperature data support for the quantification of the SPTB.

![Figure 5. Verification of the thermal model in the TMCF.](image)

### 4. Results

Based on the TMCF, the printing process of the “R” case is simulated, and the temperature field distribution and phase change distribution characteristics during the printing
process of the component area are analyzed to clarify the spatial distribution rules for the phase change. Then, referring to the phase change distribution characteristics obtained in the “R” case, the scanning power, scanning speed, hatch spacing, and evolution behavior of the precipitation phase in the characteristic area were explored according to the simulation schemes. Finally, the effect of the process parameters on the SPTB was clarified.

4.1. Temperature Field and Precipitation Evolution

Figure 6 depicts the temperature distribution within the powder bed at different times during the preparation of the IN738 superalloy using SLM under the “R” case. From Figure 6, it can be observed that when printing to different layers, the temperature distribution is similar in areas of laser loading; the rapid increase in temperature due to the high-energy laser results in the formation of a molten metal pool, transitioning the material from a powder to a solid bulk material. As the laser moves away, the molten metal pool quickly solidifies, forming solidified metal. In contrast, for the unswept region, the temperature of the material is close to the initial temperature; this is because the state of the material in this region is always a metal powder, which is less thermally conductive; thus, the temperature change is small.

Figure 6. Temperature distribution of the “R” case.

Figure 7 illustrates the distribution of the $\gamma'$ phase within the component at the end of the printing process under the “R” case. It can be seen from the figure that the $\gamma'$ phase presents the characteristic of non-uniform distribution, and its volume fraction is related to the number of printing layers and its position in the layer. Comparing the distribution of the $\gamma'$ phase volume fraction in different layers, the volume fraction from the first to the fourth layer gradually increases; from the fifth to the seventh layer, it remains unchanged; and from the eighth layer to the final layer, it gradually decreases. This result is mainly due to the fact that when the thermal cycle is applied to the first four layers, the distance between the powder bed and the substrate is relatively short, and the heat input to the powder bed is quickly dissipated to the substrate, resulting in the formation of a relatively stable high-temperature heat-affected zone in the powder bed area, which affects the kinetic coefficient of the precipitation of the phase transition and the total time for the occurrence of the phase transition. For the fifth to the seventh layer, the heat input and dissipation in the powder bed gradually reach equilibrium, forming an approximately stable heat-affected zone. The temperature histories experienced by these three layers are similar, leading to a similar history of phase precipitation. Finally, during the printing of the last three layers, the reduced cumulative time for phase transformation due to a decrease in thermal cycles leads to a decreasing trend in the volume fraction of the $\gamma'$ phase.
Figure 7. The γ′ volume fraction distribution of the “R” case.

From the analysis of phase precipitation in different regions within the layers, it can be observed that the volume fraction of the γ′ phase is positively correlated with the number of tracks, which is related to the temperature distribution characteristics of the powder bed during laser re-heating under the zigzag scan pattern. When the laser is continuously loaded, the powder bed in the area to be scanned is continuously preheated, so the amount of precipitation in these areas may increase in the phase transition temperature range.

4.2. Effect of Process Parameters on Precipitation Behavior

In the analysis of the influence of process parameters on the precipitation behavior in the process of SLM preparation of the IN738 superalloy, firstly, the effects of various process parameters on the distribution of the γ′ phase and the maximum volume fraction of the γ′ phase in the as-deposited components were compared and analyzed. Then, combined with the evolution kinetics of the γ′ phase at representative positions during the SLM, the evolution law of the precipitated phase was clarified. Finally, the internal mechanism of the influence of various process parameters on the precipitation behavior of the γ′ phase was analyzed.

4.2.1. Characteristics of the As-Deposited γ′ Phase

Figure 8 and Table 5 show the distribution of the γ′ phase and the maximum volume fraction of the γ′ phase in the as-deposited IN738 superalloy under different process parameters, respectively. Figure 8 shows that the distribution of the γ′ phase under different processing conditions resembles that of the “R” case shown in Figure 7, displaying non-uniform characteristics. Additionally, the volume fraction of the γ′ phase is influenced by the number of printing layers and the layer’s position. Further analysis of Table 5 reveals that the volume fraction of the γ′ precipitates in the material exhibits a positive correlation with the laser power and a negative correlation with the laser scanning speed and hatch spacing. A comparison between the “A2”, “B1”, “C1” cases and the “R” case demonstrates that when the laser power, laser scanning speed, and hatch spacing are altered by +50%, −25%, and −16.7%, respectively, the maximum volume fraction of the γ′ phase increases by factors of 17.377, 60.780, and 5.214, respectively. It can be inferred that when the relative changes in these three process parameters are equal, the influence on the volume fraction of the γ′ phase follows the order of laser scanning speed, laser power, and hatch spacing.
In the first stage, the precipitation and re-dissolution stage, the peak temperature of the thermal cycle of the material is higher than the temperature of the complete dissolution of the $\gamma'$ phase; at this time, the $\gamma'$ phase alternates between precipitation growth and high-temperature dissolution, its volume fraction is obtained by the superposition of the precipitation and dissolution effects, and the final value obtained is relatively small.

In the second stage, the precipitation stage, the peak thermal cycle temperature of the material is between the $\gamma'$ phase precipitation temperature interval; at this time, the $\gamma'$ phase volume fraction increases rapidly with the advancement of the printing process, but due to the increase in the number of printed layers, the peak thermal cycle temperature of the material is rapidly decaying, and the incremental increase in the volume fraction of the precipitation phase is significantly reduced.

In the final stage, the stable stage, the peak temperature of the thermal cycle of the material is small, and the kinetic coefficient of the phase transition of the material is approximated to be zero. The volume fraction of the precipitated phase of the material remains unchanged.
Table 5. The maximum volume fraction of the $\gamma'$ phase in the component after printing.

<table>
<thead>
<tr>
<th>Case</th>
<th>Laser power (W)</th>
<th>Precipitation and dissolution stage</th>
<th>Precipitation stage</th>
<th>Stable stage</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$f_{\gamma'}$ (%)</td>
<td>$t_{\gamma'}$ (s)</td>
<td>$f_{\gamma'}$ (%)</td>
</tr>
<tr>
<td>A</td>
<td>200</td>
<td>Point A</td>
<td>6.038</td>
<td>1.305 $\times 10^{-10}$</td>
</tr>
<tr>
<td>A1</td>
<td>250</td>
<td>Point A</td>
<td>1.272 $\times 10^{-3}$</td>
<td>4.020 $\times 10^{-10}$</td>
</tr>
<tr>
<td>A2</td>
<td>300</td>
<td>Point A</td>
<td>4.810 $\times 10^{-3}$</td>
<td>4.024 $\times 10^{-10}$</td>
</tr>
<tr>
<td>A2</td>
<td>300</td>
<td>Point B</td>
<td>5.024</td>
<td>2.415 $\times 10^{-10}$</td>
</tr>
</tbody>
</table>

4.2.3. Influence of the Process Parameters on the SPTB

Figure 9a,c,e illustrate the influence of laser power on the duration of the precipitation and the re-dissolution stage, the precipitation stage, and the stable stage, as well as the volume fraction of the $\gamma'$ phase at point A within the first layer during the printing process. Analysis reveals that when the laser power increases from 200 W to 300 W, the duration of the precipitation and re-dissolution stage remains at 16.008 s, while the volume fraction of the $\gamma'$ phase increases from $9.04 \times 10^{-12}$ to $4.810 \times 10^{-11}$. In the precipitation stage, the duration increases from 24.012 s to 32.016 s, increasing the volume fraction of the $\gamma'$ phase from $1.305 \times 10^{-11}$ to $6.340 \times 10^{-10}$. In the stable stage, the volume fraction of the $\gamma'$ phase remains unchanged. Notably, the magnitude of the $\gamma'$ phase volume fraction is consistent with that reported by McNamara et al. [26]. Thus, when the laser power increases from 200 W to 300 W, the volume fraction of the $\gamma'$ phase at point A experiences a significant increase, with the precipitation and re-dissolution and precipitation stages expanding by 5.321 and 48.582 times, respectively. Comparing Figure 9b,d,f, for point B in the fifth layer, when the power is increased from the “R” case to the “A2” case, the $\gamma'$ phase
volume fraction at this location increases by 11.727 and 14.037 times in the precipitation re-dissolution stage and the precipitation stage, respectively, which is an increase compared to that of the precipitation and re-dissolution stage and a decrease in the precipitation stage at point A. This is mainly because when the print changes from the first to the fifth layer, the total time that point B remains in the phase transition interval increases due to heat accumulation, and the total phase transition time increases with the increase in power, so the difference in the volume fraction of the $\gamma'$ phase in the precipitation and re-dissolution stage increases. For the precipitation stage, the decrease in the difference is related to the rapid increase in the volume fraction of the $\gamma'$ phase during the precipitation and re-dissolution stage.

Figure 10. The effects of laser scan speed on the point temperature cycles, the $\gamma'$ phase precipitation kinetics, and the volume fraction: (a,c,e) point A; (b,d,f) point B.

Figures 10 and 11 depict the influence of the scanning speed and hatch spacing on the volume fraction of the $\gamma'$ phase. Further analysis reveals that when the scanning speed or hatch spacing is reduced, point A in the first layer and point B in the fifth layer exhibit an overall increasing trend in the volume fraction of the $\gamma'$ phase during the precipitation and re-dissolution stage and the precipitation stage. The most significant increase is observed
during the precipitation stage. This outcome resembles the effects caused by an increase in the laser power. It is linked to the enhancement of laser energy density, which extends the duration that the material resides within the temperature range conducive to the $\gamma'$ phase precipitation. However, some instances defy this trend. For example, as shown in Figure 11d, when comparing hatch spacing values of 100 $\mu$m and 125 $\mu$m, the “R” case exhibits a higher volume fraction of the precipitated phase during the precipitation resorption stage. This phenomenon is primarily attributed to the interaction between the precipitation and dissolution of the $\gamma'$ phase.

**Figure 11.** The effects of hatch spacing on the point temperature cycles, the $\gamma'$ phase precipitation kinetics, and the volume fraction: (a,c,e) point A; (b,d,f) point B.

5. Conclusions

This work uses an equivalent micro-region heat source model, a non-isothermal JMA model, and the birth and death method to establish a modern phase composition prediction framework (TMCF) based on the original coupling algorithm. The TMCF can efficiently simulate the SPTB of the materials in the entire powder bed in multiple thermal cyclings during the SLM, which helps to provide insights into the evolution of the phase and the
dependence between the phase composition and process parameters, thus aiding in the achievement of a precise customization of the structure.

Taking the IN738 superalloy as an example, it was found that the \( \gamma' \) phase distribution after printing exhibits a non-uniform distribution, and the distribution was related to the number of printed layers and the positions within the layer, and the results can be applied to other MCPA. Specifically, with the increase in the number of printed layers, the volume fraction of the precipitated phase shows a trend of increasing first, then becoming approximately constant, and finally decreasing; when the number of tracks is increased from the one to five, the volume fraction of the precipitated phase is approximately positively correlated with the number of tracks.

To clarify the reasons for the phase distribution characteristics, we studied the evolution of the \( \gamma' \) phase and discovered an interesting and novel SPTB. Specifically, the transformation of the \( \gamma' \) phase can be divided into three stages according to the cycling temperature and SPTB: the precipitation and re-dissolution stage, the precipitation stage, and the stable stage. Among them, the precipitation and re-dissolution stage of the material undergoes a higher temperature; there is an interaction between the two phenomena of precipitation and re-dissolution, while during the precipitation stage in regards to the temperature of the material, only precipitation behavior occurs, and the \( \gamma' \) phase volume fraction increases to a relatively large extent; for the stable stage, the volume fraction of the \( \gamma' \) phase remains unchanged. Hence, the non-uniform phase distribution can be primarily attributed to significant variations in the temperature history across different spatial locations.

Ultimately, we quantitatively estimated the dependence of the obtained phase composition on the SLM mode, and the dependencies may help to optimize the SLM mode, to obtain high-quality components, to develop new preparation processes, and to regulate the phase composition to avoid SAC. Specifically, when the laser power, laser scanning speed, and hatch spacing are altered by \(+50\%\), \(-25\%\), and \(-16.7\%\), respectively, within the process window, the maximum volume fraction of the \( \gamma' \) phase increases by factors of \(17.377\), \(60.780\), and \(5.214\), respectively. It can be inferred that when the relative changes in these three process parameters are equal, the influence on the volume fraction of the \( \gamma' \) phase follows the order of laser scanning speed, laser power, and hatch spacing.

However, this work and the TMCF exhibit certain limitations, such the fact that the scale used has not yet broken through the mesoscopic scale, and the development of multi-scale coupling algorithms is required to realize the simulation of the phase composition of the macroscopic products. In addition, many metals have difficulty undergoing significant diffusion SPTB due to the rapid cooling rates within the traditional SLM process window. Therefore, this work uses mainly the TMCF model to theoretically study the evolution of the precipitated phase and its relationship with the process parameters from a simulation perspective.

In the future, our team will combine novel strategies, such as multi-laser in situ heat treatment, substrate preheating, complex scanning paths, and other strategies, with the experimental work and the results of this study to provide the possibility of fully utilizing the potential of the SLM process to obtain high-quality products.

**Author Contributions:** Conceptualization, H.K. and Z.B.; methodology, H.K., Y.H. and H.Q.; software, H.K. and J.X.; validation, H.K. and H.Q.; formal analysis, H.K. and H.Q.; resources, Y.H. and J.X.; data curation, H.K. and Y.H.; writing—original draft preparation, H.K.; writing—review and editing, H.S. and Z.B.; supervision, H.S. and Z.B.; funding acquisition, H.S. All authors have read and agreed to the published version of the manuscript.

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