On the dendrite growth simulation during multitrack selective laser melting process

A V Dubrov 1, F Kh Mirzade 1, V D Dubrov 1
1ILIT RAS – Branch of the FSRC «Crystallography and Photonics» RAS,
Svyatozerskaya 1, 140700, Shatura, Moscow Region, Russia

Abstract. The evolution of the microstructure in the selective laser melting (SLM) process is investigated in the framework of a multiscale approach. The kinetic equation for the phase-field (order parameter) coupled with the energy transfer equation is used to describe the crystallization processes. To study the effect of technological parameters on the microstructure of the synthesized product, and to establish a connection between the models of macro- and micro-scale through the temperature gradient, numerical studies of macro processes in the formation of a series of parallel SLM tracks were carried out. It is shown that the adjustment of the laser power level changes the temperature dynamics in the test areas, which, in turn, through the changed temperature gradients affects the evolution of the microstructure in the micro-scale model. The calculations showed that the implemented numerical model qualitatively describes the kinetics of crystallization and formation of microstructures in the SLM process.

1. Introduction
Additive manufacturing (AM) has received increased attention in recent years because of its ability to produce parts directly from CAD data [1]. Selective laser melting (SLM) is a method of AM, in which the creation of a metal part is carried out through the layer-by-layer addition of powder materials. The SLM process uses a high-intensity laser source to create a melt pool in the powder layer. The process flow is determined by a large number of factors such as laser beam power, laser spot size, scanning speed and strategy, powder layer thickness, particle shape and distribution function, powder physical and chemical properties, etc. It should be noted the relationship of factors affecting the process and the presence of many interacting processes: the absorption and scattering of laser radiation by powder particles, heat conduction and convection, the evolution of the free surface of the melt due to capillary forces, evaporation, shrinkage, crystallization, the formation of the microstructure of the synthesized object [1].

From numerous experiments it is well known that a variety of microstructures (columnar, cellular, dendritic, cellular-dendritic), arising at the stage of crystallization in SLM, and the mechanisms of their formation and changes largely determine the physical and mechanical characteristics of the synthesized product. At the same time, the use of a single direct numerical simulation of dendritic crystallization to predict the properties of the material presents serious difficulties. The main problems here are related to the description of the complex interaction of nonlinear processes occurring at different scale levels. Recently, new directions of research concerning multilevel (two-level) models are emerging, considering jointly the processes at different scale levels: micro- and macro-levels [2]. In [3], a physical and mathematical model of the dynamics of the liquid-solid phase boundary movement and prediction of the microstructure in the SLM of the powder compact using a two-level (macroscopic–microscopic) approximation was developed.
In this paper, the growth dynamics and morphology of columnar dendritic structures are numerically investigated. For this purpose, the simultaneous growth of several crystallites under temperature gradient is considered. In addition, to establish the connection of macro- and micro-scale models through a local temperature gradient, numerical studies of macro processes in the formation of a series of parallel SLM tracks were carried out.

2. Numerical simulation of the evolution of the microstructure

The evolution of the microstructure (micro-level) is described by the phase-field method, which relies on the use of a differential equation for the order parameter coupled with the equations of thermal conductivity [3]. The phase-field model is very effective in the description of nonequilibrium dendritic evolution. In numerical studies based on them, all control equations are written for the entire region without separating the interface from the solid and liquid phases and no direct tracking of the interface position is required. Simulation of solidification in SLM by the phase-field method involves the growth of grains in the supercooled liquid phase. According to this hypothesis, it is necessary to take into account three regions: a crystalline nucleus, a liquid phase, and a solid / liquid interface.

We introduce the characteristic of the phase state of matter - the phase-field: \( \phi(r,t) \). A variable \( \phi(r,t) \) can be interpreted as the degree of orderliness of a material in a microvolume with a radius vector \( r \) at time \( t \). The phase-field variable \( \phi = 0 \) for liquid, and \( \phi = 1 \) for solid and varies smoothly between those values over the solid–liquid interface, so \( \phi \in (0,1) \) in the diffuse interface. The evolution of the microstructure is modeled by the kinetic equation (1) for the phase field (\( \phi \)), which is coupled with the heat equation (2)

\[
\tau \phi = e_0^2 \nabla \cdot \left[ \hat{e}(\theta)(\hat{e}(\theta)I + \hat{e}'(\theta)I) \cdot \nabla \phi \right] - \omega_s g'(\phi) + 30g(\phi)\left[ L_0 \left(1/T - 1/T_m \right) \right],
\]

\[
\phi_T = \hat{c} \nabla^2 \phi - \left[ p'(\phi)L_0 + \omega_s g' \phi \right] \phi,
\]

\( m_{\phi} = \tau^{-1} \) is the mobility of the phase boundary, \( L_0 \) and \( T_m \) are the heat of fusion and melting point, respectively. The constant \( \omega_s \) characterizes the height of the energy barrier between phases: \( \omega_s = 3\sigma/\sqrt{2}T_m\delta \) (\( \sigma \) is the surface energy, \( \delta \) is the width of the front of the phase transition), \( \alpha^2 = 6\sqrt{2}\sigma\delta/T_m \) characterizes the width of the diffuse interface, \( \delta = \epsilon/\sqrt{4\sigma} \), \( \chi = MT^2 \) is the thermal conductivity, \( \epsilon \) is the heat capacity, \( \epsilon \) is the coefficient taking into account the anisotropy of the surface energy: \( \epsilon = \epsilon_0 \hat{e}(\theta) \) (\( \epsilon_0 > 0 \)). The variable \( \theta \) is the angle between the x-axis and the normal vector of the interface \( n = \nabla \phi \). For 2D geometry: \( \hat{e}(\theta) = 1 + \alpha \cos 4\theta \), \( \theta = \arctan[\partial \phi/\partial y/\partial \phi/\partial x] \) [4]. The interpolation functions \( g(\phi) = \phi^5(1-\phi)^2 \) and \( p(\phi) = \phi^6 \left(10 - 15\phi + 6\phi^2 \right) \) are chosen in such a way as to provide a description of the interface of a finite width (the free energy potential has minima at \( \phi = 0 \) and \( \phi = 1 \)).

The formation of the crystal structure of the material occurs as a result of the formation and growth of a set of crystalline nuclei. The rate of crystal formation is determined by the local degree of supercooling. Depending on this, the number of simultaneously growing crystallites in this area may vary. Materials obtained by laser AM characterized by high temperature gradients and high cooling rates. The most typical microstructure in AM of austenitic stainless steel is the cellular structure and columnar dendrites [5].

This section numerically studies the growth dynamics and morphology of columnar dendritic structures. For this purpose, the simultaneous growth of several crystallites under temperature gradient is considered. The development of several crystallites in the adjacent space leads to their competition [6]. If their crystallographic orientation is close, then due to the close location only the lateral branches are suppressed, and the primary branches grow in a parallel direction, forming a columnar structure. A
constant value of the temperature gradient was used, a fixed value of dimensionless supercooling $9 \times 10^{-4}$ was set at the left boundary and $7 \times 10^{-4}$ at the right boundary. These values are typical for the SLM process of metallic materials. Iron-specific data were used as material properties.

Calculation of dendritic microstructures was carried out in a two-dimensional area of $15 \times 15$ microns, which was divided into 2000 cells in each dimension. The total number of calculated cells in the mesh was 4 million. Before the start of the calculation, round “crystallites” with a radius of 8 cells were placed in the required places of the calculated area. A static dimensionless time step was used, equal to $0.5 \times 10^{-3}$. To carry out calculations in parallel, the spatial domain was decomposed into 16 subregions. The duration of the calculation was about 2 hours.

Figure 1 shows the development of six crystallites uniformly placed at the initial time on the lower boundary of the computational domain. Evolution within 30 µs is demonstrated, which corresponds to the value of the dimensionless time 0.6. The color indicates the temperature distribution. Due to the dense packing of crystallites, almost complete suppression of the growth of secondary branches occurs, and a columnar microstructure develops. In the conditions of temperature gradient the difference in growth rates is observed. The development of dendrites, which are at a greater supercooling closer to the left border, is ahead of structures in less favorable conditions.

The morphology of columnar dendrites obtained by simulation qualitatively correspond to that observed in experiments, for example [7]. The calculations have shown that the numerical model qualitatively describes the physics of crystallization and formation of microstructures in the SLM process.

3. Influence of macro-conditions on microstructure development
To link the macro- and micro-scale models, the temperature gradient used in the calculation of the microstructure evolution can be taken from the corresponding sub-domain of the macro-scale. To study the effect of technological parameters on the final quality of the synthesized product, parametric studies of macro processes were carried out in the formation of a series of parallel SLM tracks. SS304L stainless steel data were used as substrate and powder material properties.

Figure 2 shows the temperature dependences in the test areas when scanning three parallel tracks for two laser power levels. The temperature measurement test areas are located at the substrate level in the middle of the respective tracks. The temperature peaks on the graphs correspond to the moments of the beam passing through the corresponding points. Each region experiences 3 heating-cooling cycles, which indicates that the material is subjected to cyclic processes of temperature change, which can lead to high residual stresses [8]. With the use of higher power, there is a slight increase in the maximum achievable temperature at the time of passage of the laser beam through the temperature measurement area (about 50-100 degrees). At the same time, the temperature drop occurs with a delay of about
1-1.5 ms. Preheating of the material during the processing of adjacent areas also increases by 50-100 degrees, but the dynamics of heating to melt point does not change. Also, the heating pattern of the first track and the subsequent ones, the material of which was preheated, does not differ. It is shown that the adjustment of the laser power level changes the temperature dynamics in the test areas on the substrate surface, which, in turn, through the changed temperature gradients will affect the calculation of the microstructure evolution in the micro-scale model.

![Figure 2](image-url)

**Figure 2.** Evolution of the temperature in the test areas when scanning three parallel tracks with different laser power: dashed line – 200 W; solid line – 300 W. Process parameters: scanning speed 60 mm/s, the thickness of the powder layer 130 microns, the distance between the tracks 154 microns, particle size distribution 40-100 microns.

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