Phase field simulation of dendrite evolution during powder-based laser metal deposition

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Abstract. An algorithm for simulation of laser metal deposition (LMD) processes is developed, which implements the concept of multi-scale modeling of crystallization. The macro-level model takes into account the coupled dynamics of the free surface (melt-gas) and the energy and mass transfer of the multiphase mixture, which is applied on scales of the order of a few to tens of millimeters. The micro-level model describes the evolution of dendritic structures using the phase-field method (PFM) at scales of the order of a few to tens of micro-meters. Wherein, the resulting macroscopic temperature distribution in the system defines the boundary and initial conditions of the micro-model, which, in turn, control the growth patterns and evolution of the dendrites. In local sub-region, the evolution of the dendrite in an advantageous position was simulated, i.e. having favorable thermodynamic conditions of its growth. Before solving the micro-scale problem with the PFM, the 3D mesh conversion procedure to the new 2D mesh is performed in the sub-region of interest. To do this, we select the plane in which the local temperature gradient vector lies. The test dynamic profiles of the phase field and temperature in different spatial regions of the formed bead are calculated. Simulations used the values of physical quantities for iron. The results of calculations showed that the developed numerical model qualitatively describes the physics of crystallization and the formation of dendrites in the LMD process. The effect on the growth dynamics of dendritic structures of such PFM parameters as thermal noise and the anisotropy amplitude is analyzed. It is shown that thermal fluctuations strongly affect the branching of dendrites. With an increase in the fluctuation amplitude, the phase boundary becomes unstable with the formation of secondary and tertiary branches.

1. Introduction
Currently, an advantageous and promising component of modern production is the laser additive manufacturing (AM) of metal powder parts. One of the important additive methods of product synthesis is laser metal deposition (LMD) [1]. The micro-structure of the material plays a decisive role in determining the physical and mechanical properties of the final product synthesized by AM [2]. Control and optimization of the micro-structure is one of the important issues in the development of new materials and technologies. Micro-structures establish the main length scales that affect the properties of materials. However, according to current literature there is no uniform approach to predicting the length scales and micro-structure as a function of processing and AM parameters.

A characteristic feature of laser AM is the interaction of many different phenomena. These include: absorption and scattering of laser radiation by the substance of the substrate and powder particles, the propagation of heat and melting of the metal, the formation of a free surface of the melt under the action of powder pressure and capillary (including thermo-capillary) forces. Crystallization processes occur
under conditions of large temperature gradients and cooling rates, stresses and deformations, which indicates the non-equilibrium nature of the processes under consideration.

Selection of process parameters values by trial and error is a time-consuming and costly process. Therefore, when choosing the operating ranges for parameter values, it is promising to use a comprehensive numerical model of the AM process. However, the fundamental complexity in the construction and use of such AM model is the difference in spatial and temporal scales on which heat-mass transfer and micro-structure processes occur.

Fluid flows and heat transfer in the LMD process have been studied in a number of works, for example [3, 4]. However, the modeling of the evolution of the micro-structure of solidification in the LMD process is still not sufficiently developed. Stefan's classical approach to modeling solidification involves tracking the boundary separating the two phases. This requires solving the equations in each phase, while maintaining the boundary conditions for such quantities as temperature or concentration and their derivatives at the moving interface. The numerical methods required for explicit interface tracking are often complex and numerically inefficient. Over the past decades many theoretical approaches to the formation of a micro-structure in the process of phase transition have been developed. The most recent approaches are the phase field method [5, 6] and the methods of cellular automata [7]. Phase-field models replace mathematically sharp interfaces with diffuse ones and avoid explicit tracking of the interface.

In this paper, an algorithm is developed for calculating processes during LMD that implements the concept of multiscale modeling of crystallization. The effects of macro-processes, as well as such parameters of PFM as thermal noise and the anisotropy amplitude, on the growth dynamics of dendritic structures were studied.

2. Algorithm of multiscale problem
The developed algorithm for solving the multiscale problem of LMD modeling has a modular architecture. The general structure of the multiscale algorithm is presented in figure 1. The algorithm consists of a module for calculating the macro-level model; module that calculates the evolution model of the micro-structure; and a module that provides scales communications.

The macro-level model takes into account the coupled dynamics of the free surface (melt-gas) and the energy and mass transfer of the multiphase mixture, and is applied on scales of the order of a few to tens of millimeters [8]. In this case, heat transfer, convective thermo-capillary movement of the melt, and addition of the mass of the powder to the fusion zone are taken into account in a self-consistent manner. The micro-level model [9] describes the evolution of dendritic structures using the phase-field method (PFM) at scales of the order of a few to tens of micro-meters. Wherein, the resulting macroscopic temperature distribution in the system defines the boundary and initial conditions of the micromodel, which, in turn, control the growth patterns and evolution of the dendrites.

In the macro-scale module, the procedure for calculating the micro-scale model is initiated by calling the scale communication module. For this, the launch criterion is formulated. In this implementation of the algorithm, a criterion was set for the parameters of the formed bead to enter the stationary regime: the dimensions of the melt pool and the height of the bead. In the general case, the criterion can be the conditions for the existence of any anomalies of the thermal field. For example, associated with working out the complex elements of the part construction trajectory. Either other conditions associated with the possibility of forming micro-structures, the parameters of which need to be controlled by the end user of the developed software.

The scale communication module prepares the input data necessary for the calculation of the micro-scale, based on the information of the upper level. It localizes the two-phase zone (liquid-solid), and allocates sub-regions for calculating the micro-scale model from the calculated macro-level region in the phase transition zone. Then the conversion of the selected areas of the macro-scale is performed to solve the PFM equations. To do this, the spatial orientation of the new 2D mesh is determined, the values of the macroscopic temperature distribution are projected onto the calculated area of the micro-scale, and interpolation of values and the calculation of a new undercooling field are performed.
During the solidification in LMD, the effect of the competitive growth of crystalline grains appears. In this case, favorable conditions arise for the growth of grain, whose crystallographic orientation more closely corresponds to the direction of the local gradient of the macroscopic temperature field. Such grains outstrip the growth of grains with other crystallographic orientations, block the development of grains that are in less favorable conditions and gradually displace them [10].

In each local sub-region, the growth of the dendrite in an advantageous position was simulated, i.e. having favorable thermodynamic conditions from the point of view of its growth. The first-order axis of such a dendrite is oriented along the direction of the local temperature gradient. It is assumed that the crystallization of a material with a cubic face-centered crystal (FCC) lattice is modeled, which is true for many pure metals and alloys of practical interest (Fe, Ni, steel, etc.).

The growth of the dendrite in the material with the FCC crystal lattice from the undercooled melt demonstrates the octahedral shape, which was shown in the experiment [11] and in the simulation [12]. Developing in a homogeneous temperature field, crystallites have the shape of a regular octahedron, the growth rate along all diagonal directions is equal. In the presence of inhomogeneity in the temperature field, local growth conditions change, the phase-field profile loses symmetry. The growth of the dendrite predominates in the direction of the heat outflow.

Before the solution of the micro-scale problem, the 3D mesh conversion procedure is performed in the macro-space sub-domain of interest to the new 2D mesh for calculating the PFM (see figure 2). To do this, a plane in the local subdomain is chosen such that the local temperature gradient vector lies in it. In this plane, a new mesh is constructed for the micro-scale model, with its division into cells being performed in parallel and orthogonal to the temperature gradient. Owing to the smallness of the region for calculating the micro-scale, the front of the temperature distribution is assumed to be flat. In this case, the local temperature field will not have singularities leading to a non-uniform growth of the dendrite in the direction transverse to the temperature gradient. Then, taking into account the octahedral shape of the dendrite, up to the angle of rotation around the direction of the temperature gradient, to obtain a flat section of the dendrite we choose a plane passing through the central trunk and two
secondary branches. The perpendicular section passing through the trunk and the other two secondary branches will in this case be equivalent, and for 3D representations can be obtained by rotating the calculated profile 90° around the trunk.

The initial distribution of the temperature field is established in accordance with the data obtained from the macro-scale model. Values are interpolated on a new mesh taking into account its spatial orientation. In the center of the calculation area, a circular "crystallite" with a fixed radius is placed. In the cells occupied by the "crystallite", the order parameter field assumed the value 1, the rest of the space was filled with a zero value.

![Figure 2. Scheme for the conversion of the macro-scale sub-region to calculate the phase-field model.](image)

The PFM equations are solved on separate computing resources. When starting a micro-scale model, the calculation of a macro-scale model is not interrupted in order for information to be available at the end of the calculation both about the geometric and heat-hydrodynamic characteristics of the process, as well as the micro-structure data in one or several sub-regions.

In the module for calculating the micro-scale, a sequential solution of the phase field, energy and composition equations, as well as the addition of random thermal noise, is carried out at each time step. Stochastic noise is an important component of PFM for crystallization, which describes the pronounced effect observed in practice. Random thermal fluctuations are a factor affecting the stability of the phase boundary, and the cause of branching with the formation of secondary and tertiary branches of dendrites [13]. Noise calculation is necessary to obtain realistic results. This can be done in the form of an additive term in the phase-field equation or the energy equation. Adding a component is done in the area occupied by the boundary cells in the entire calculated volume. The noise is added in the form of an expression $a_{\text{noise}}(1-\phi)\chi_{\text{noise}}$ to the right side of the energy equation, where $a_{\text{noise}}$ is the amplitude of the noise component, and $\chi_{\text{noise}}$ is a random variable uniformly distributed in the interval [-0.5, 0.5] [14].

At the boundaries of the calculated volume, the zero value of the gradient of the corresponding quantity was fixed for the phase field, temperature, and composition. The equations of the model were discretized by the finite volume method. To find a discrete analogue of the differential equations of the model, each term of the equation is integrated into a control volume. For the discretization of temporal derivatives, an implicit Eulerian first order scheme was used. The derivatives in space were discretized according to the scheme of central differences. The obtained systems of linear algebraic equations were solved by the conjugate gradients method (PCG), with preconditioning by the block incomplete Cholesky factorization.
3. Numerical simulation procedure, results and discussion

The software implementation of the multiscale algorithm is in the paradigm of object-oriented programming using the OpenFOAM 2.4 utilities and C++ class library for numerical simulation. For numerical realization of the macro-scale algorithm, a block-structural hexahedral mesh consisting of ~0.8 million cells was used. The computational volume size is 16x10.8x9.9 mm. The size of the cells in the detailed region is ~50x50x48 μm. A more detailed description of the methodology for calculating the macro-scale problem is given in [15]. To calculate the micro-scale model, physical sub-regions of 15*15 micron size were considered. In each sub-region, the evolution of the micro-structure over 40 μs was investigated. An orthogonal mesh consisting of 4 million cells (2000x2000) was used. For the mesh used, the size of one computed cell is 7.5*7.5 nm. Before starting the calculation, a circular "crystallite" with a radius of 5 calculated cells is placed in the center of the calculation area.

Test calculations of a multiscale model of the micro-structure evolution during the LMD were carried out for the task of forming a single bead. The properties of the materials of the deposited powder and the substrate were used to characterize the data for iron. Parametric studies of the influence of PFM control parameters, as well as parameters of the technological process, on the development of micro-structural features of the material were carried out. Dynamic profiles of the phase field and temperature in different spatial regions of the formed object are calculated.

The laser radiation power was varied within the range (0.800-1.6) kW, and the scanning velocity was within (3.5-7.5) mm/s. The remaining parameters of the technological process maintained constant. The values of the physical quantities for iron are taken from [16]. Local thermal conditions (the distribution of the initial undercooling field), in which the development of the micro-structure was modeled, were taken from the solution of the upper-level model. The dimensionless values of the anisotropy amplitude (δ) varied in the range 0.01-0.06, and the thermal noise amplitudes (a_th) in the range 0-0.1·10^-3. Complete data on the used values of physical quantities, process parameters and PFM control parameters are given in [17].

The values of the local temperature gradient vary depending on the location of the sub-region of the PFM calculation within the macroscopic region, as well as on the parameters of the technological process, thereby influencing the development of the local micro-structure. To study the evolution of the micro-structure, three sub-regions were chosen in the solidification zone at the rear of the melt pool. The location of the sub-regions is indicated by the parallelepipeds in figure 3. Two vertical cross sections of the melt pool are located, which are parallel to the scanning direction. One of them passes through the axis of the laser radiation and, accordingly, the center of the melt pool, the second - displaced by 2.5 mm to the side edge of the bead. In each of these cross sections, a sub-surface sub-region located 100 μm below the local level of the surface at the rear wall of the melt pool (regions 1 and 3) is considered. In addition, a sub-region located on the rear bottom wall of the melt pool (region 2) is also considered in the central section.

Figure 3 shows the resulting spatial morphology of dendrites developing in three sub-regions of the solidification zone. The contours denote the longitudinal vertical cross-sections of the melt pool with the indication of directions of the local temperature gradients. To obtain a 3D image of dendrites, the calculated 2D phase field profiles are presented on two mutually perpendicular planes containing a local temperature gradient vector.

The graphs (see figure 4) show the dependence of the absolute values of temperature gradients in the three considered subareas on the value of the linear energy density. Values are obtained after building a 5 mm long bead. The magnitude of the linear energy density is considered in order to use a uniform approach to the analysis of temperature gradients when varying the parameters of the technological process. It is defined as $\overline{T} = \frac{P_{las}}{V_{scan}}$, where $P_{las}$ is the laser radiation power, and $V_{scan}$ is the scanning velocity.

The values in regions 1 and 3 have a wide spread, which is explained by the strong dependence of the temperature gradient on the shape of the melt pool and the local dynamics of the liquid. The dynamics of the liquid phase in the melt pool under the action of laser radiation and the gas-powder flux is highly
unsteady. The values of the temperature gradient in sub-region 2 depend weakly on the energy density. This region is located at the lower back boundary of the melt pool, farther from the radiation absorption zone than regions 1 and 3. Hydrodynamic currents formed by surface thermo-capillary forces have a more moderate influence here than in the near-surface subareas 1 and 3.

![Figure 3](image)

**Figure 3.** The spatial morphology of dendrites developing in three sub-regions of the solidification zone. The contours denote the longitudinal vertical sections of the melt pool with the directions of the local temperature gradients. Process parameters: P = 1600 W, Vs = 3.5 mm/s.

![Figure 4](image)

**Figure 4.** Dependence of temperature gradients on the linear energy density in three sub-regions.

The effect on the growth dynamics of dendritic structures of such PFM parameters as thermal noise and the anisotropy amplitude was analyzed. A temperature gradient of 2400 K/mm was used. Figure 5 shows the phase profiles of the dendritic structures obtained for different values of the PFM control parameters (dimensionless time value $\tilde{t} = 0.4$). The color indicates the temperature distribution. It is seen that, because of the presence of a temperature gradient and inhomogeneous growth conditions, the profile of the phase field loses symmetry. There is a faster growth of the left side of the dendrite, corresponding to the direction of the prevailing heat outflow.

Random thermal fluctuations are a factor affecting the stability of the phase boundary, and the cause of branching with the formation of secondary and tertiary branches of dendrites. The calculation of thermal noise is necessary to obtain realistic results. Based on the results of the simulation, it is shown that thermal fluctuations strongly affect the branching of dendrites. With an increase in the fluctuation amplitude, the phase boundary becomes unstable with the formation of secondary and tertiary branches. To a greater extent, the effect of thermal noise on the morphology is manifested for the value of the dimensionless anisotropy amplitude $\delta = 0.06$.

An increase in the values of the anisotropy amplitude leads to a pronounced growth in the chosen directions. For the iron with FCC lattice used in the calculation the symmetry value $j = 4$ is used, which causes the resulting shape. With an anisotropy amplitude of 0.01, the shape of the obtained dendrite is close to a square one, which corresponds to the cross section of the octahedron through four vertices.
lying in one plane. The square shape is changed, due to the induced inhomogeneity of the thermal field and the corresponding stimulation of directed growth.

In figure 5(d), the characteristic effect of competitive growth of dendrite branches is clearly visible. The secondary branches on the left side of the dendrite, which are in more favorable thermodynamic conditions, show a rapid growth in the vertical direction. They block the development of third-order branches growing in the horizontal direction. On the right side of the dendrite, the opposite effect is observed when the vertical secondary branches are poorly developed and will soon be blocked by horizontal branches.

![Figure 5](image)

**Figure 5.** Profile of the phase field of dendritic structures and temperature distribution. The dimensionless value of time $\tilde{t}$: 0.4. Amplitude of thermal noise $a_{\text{nd}}$: 0.0; 0.1·10^{-3}. Anisotropy amplitude $\delta$: 0.01; 0.06.

### 4. Conclusion

This paper describes the developed algorithm for laser metal deposition (LMD) simulation that implements the concept of multiscale modeling of crystallization. The macro-level model takes into account the coupled dynamics of the free surface (melt-gas) and the energy and mass transfer of the multiphase mixture, which is applied on scales of the order of a few to tens of millimeters. The micro-level model describes the evolution of dendritic structures using the phase-field method (PFM) at scales of the order of a few to tens of micro-meters. A method for constructing a micro-scale mesh is implemented taking into account local thermal conditions found from the macro-scale model. The macro-scale data is used as the boundary and initial conditions for calculating the micro scale model. Thus, through the macro-level, a relationship is established between the parameters of the technological process and the conditions for the formation of the micro-structure of the material.
The test dynamic profiles of the phase field and temperature in different spatial regions of the formed bead are calculated. Simulations used the values of physical quantities for iron. The results of calculations showed that the developed numerical model qualitatively describes the physics of crystallization and the formation of dendrites in the LMD process. The effect on the growth dynamics of dendritic structures of such PFM parameters as thermal noise and the anisotropy amplitude is analyzed. It is shown that thermal fluctuations strongly affect the branching of dendrites. With an increase in the fluctuation amplitude, the phase boundary becomes unstable with the formation of secondary and tertiary branches.

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