

# The Study on Simulation Theory of Solidification Microstructure of Alloy Melt Pool in the Laser Additive Manufacturing Process

Yue Zhou<sup>a</sup>, Suiyuan Chen<sup>b,\*</sup>, Tingting Guan<sup>c</sup>, Tong Cui<sup>d</sup>, Jing Liang<sup>e</sup>,  
Changsheng Liu<sup>f</sup>

Key Laboratory for Anisotropy and Texture of Materials(Ministry of Education),  
School of Materials and Engineering, Northeastern University, Shenyang 110819, China

<sup>a</sup>yuezhou93@sina.com, <sup>b,\*</sup>chensy@atm.neu.edu.cn, <sup>c</sup>tingtingguan@sina.com

<sup>d</sup>cui t@smm.neu.edu.cn, <sup>e</sup>Liang j@atm.neu.edu.cn, <sup>f</sup>csliu@mail.neu.edu.cn

**Keywords:** Laser additive manufacturing; alloy steel; microstructure of melt pool; phase field method; cellular automaton method.

**Abstract:** With the development of laser additive manufacturing technology (LAM) and computer technology, it has been widely concerned that the simulation method is used to predict the solidification microstructure of alloy melt pool in the LAM process, because simulation method has advantages of short experimental period, low cost and comprehensiveness. This paper respectively introduces the basic principle of phase field (PF) model and cellular automaton (CA) model, and then illustrates the application of simulating the solidification microstructure of alloy melt pool in the process of LAM. In addition, the results of comparative analysis shows that CA method is more suitable for simulating the microstructure of melt pool than PF method in the LAM process. Finally, the existing problems and future development trends of models and algorithms are put forward, which provides a theoretical reference for the laser additive manufacturing of alloy steel.

## 1. Introduction

The basic principle of Laser additive manufacturing (LAM) is ‘Discrete and Stacked’. It is a kind of direct manufacturing technology which uses alloy powder or wire material as raw material, combined with laser metallurgy/rapid solidification. Compared with the traditional technology, it has the advantages of short production circle, high utilization ratio of materials and low cost. More importantly, the solidification process of alloy melt pool greatly deviates from the equilibrium, so the micro-sub-structure in the crystal is significantly refined and the new metastable phase even amorphous may appear, which means that the solidification microstructure of the melt pool determines the comprehensive properties of forming material to a large extent [1].

The traditional experimental method has many problems such as long study period, high cost and insufficient consideration. With the development of computer technology and solidification theory, it is possible to quantitatively simulate the solidification process and to predict the microstructure by using mathematical models. Accordingly, it will be easier to optimize the technological parameters of LAM, and then to produce metal components with ideal microstructure [2].

Based on the LAM, using 12CrNi2 alloy steel materials to produce the nuclear power emergency diesel engine crankshaft and 24CrNiMo alloy steel materials to produce the brake disc of high-speed rail are capable of improving the comprehensive mechanical properties. However, at home and abroad, the microstructure simulation of alloy melt pool in the LAM process is limited to titanium alloy, superalloy and stainless steel. Therefore, according to the existing theories and algorithms, a model can be proposed to simulate the microstructure of alloy steel melt pool. At present, there are two main methods for simulating the microstructure of melt pool: phase field (PF) method and cellular automaton (CA) method. This paper introduces the basic principle of PF model

and CA model, and then illustrates the application of simulating the solidification microstructure of alloy melt pool. Furthermore, the problems and the future development direction in simulating the solidification microstructure of melt pool are put forward.

## 2. Simulation of Solidification Microstructure of Alloy Melt Pool Based on Phase Field Method

### 2.1 Fundamental Theory of Phase Field Model

The solidification simulation of metal materials is defined as a time and space description of the moving solid/liquid interface. The PF method simulates the phase type by solving governing differential equations which describe the phase field evolution of pure metal or multi-component alloys. While the CA method simulates the dendrite morphology by determining the solid/liquid interface on the basis of the temperature field and solute field [3].

The PF model is based on the Ginzburg-Landau theory, and the physical state of the solidification interface is tracked by introducing the phase parameter  $\varphi(r, t)$ . Sun et al. [4] in Hunan University proposed a developed model as follows:

$$\begin{aligned} \tau_0 a^2(\theta) \frac{d\varphi}{dt} = & W_0^2 \nabla[a^2(\theta) \cdot \nabla \varphi] + [\varphi - \lambda \cdot u \cdot (1 - \varphi^2)] \cdot (1 - \varphi^2) \\ & - \frac{\partial}{\partial x} [W_0^2 \cdot a(\theta) \cdot a'(\theta) \frac{\partial \varphi}{\partial y}] + \frac{\partial}{\partial y} [W_0^2 \cdot a(\theta) \cdot a'(\theta) \frac{\partial \varphi}{\partial x}] \end{aligned} \quad (1)$$

where  $\varphi=1$  represents the solid phase,  $\varphi=-1$  represents the liquid phase, and the phase field variable  $\varphi(r, t)$  changes abruptly and continuously in the range of  $-1 \sim 1$  at the solid/liquid interface,  $\tau_0$  is the time of atomic motion,  $W_0$  is the thickness of the solid/liquid interface,  $\lambda$  is the coupling coefficient for the temperature field and the phase field;  $\theta = \arctan(\frac{\varphi_y}{\varphi_x}) - \theta_n$ , where  $\theta$  is the angle between the normal direction and the solid/liquid interface,  $\theta_n$  is the angle between the temperature gradient direction and the  $x$  axis;  $a(\theta) = \gamma \cdot \cos 4\theta + 1$ , Where  $\gamma$  is the coefficient of anisotropy.

### 2.2 PF Simulation Method of Solidification Microstructure of Alloy Melt Pool

The PF model is combined with the finite element analysis method (FEA) to solve the equations above. Fallah et al. [5] used the thermal analysis model in the process of direct laser deposited Ti-Nb alloy as follows:

The laser beam intensity is a Gaussian distribution:  $I_r = \frac{2P}{\pi R_b^2} \exp(-\frac{2r^2}{R_b^2})$ , where  $P$  is the laser power,  $R_b$  is the radius of laser beam,  $r$  is the distance from the center of laser beam. The temperature distribution of the substrate and the deposited material is determined by solving the three-dimensional transient heat conduction equation:

$$\frac{\partial}{\partial x} (k \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (k \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (k_t \frac{\partial T}{\partial z}) + Q_l = \frac{\partial(\rho C_p T)}{\partial t} \quad (2)$$

where  $k_t$  is the thermal conductivity,  $Q_l$  is the energy produced per unit volume,  $C_p$  is the specific heat capacity, the unit is  $J/g \cdot K$ ,  $\rho$  is the density, the unit is  $g/m^3$ .

At the initial time, the temperature of the substrate and the deposition layer is  $T_0$ , which is expressed as (3), (4):

$$T(x, y, z, 0) = T_0 \quad (3)$$

$$T(x, y, z, t_{activation}) = T_0 \quad (4)$$

where  $T_0$  is the room temperature,  $t_{activation}$  is the time it takes to add the deposited material to the system. In addition, considering the influence of moving laser beam on the boundary condition of substrate region, the boundary equation is as follows:

$$k_t (\nabla T \cdot n) = [\beta_l I - h(T - T_0) - \varepsilon_R \sigma_R (T^4 - T_0^4)] \quad (5)$$

where  $n$  is the normal vector of the surface,  $\varepsilon_R$  is the emissivity,  $h$  is the coefficient of heat convection,  $\sigma_R$  is Stefan-Boltzmann constant ( $\sigma_R=5.67 \times 10^{-8} \text{ W m}^2 \text{ K}^4$ ),  $\beta_I$  is the absorption factor of laser power,  $I$  is the energy density distribution of substrate, the unit is  $\text{W/m}^2$ .

### 3. Simulation of Solidification Microstructure of Alloy Melt Pool Based on Cellular Automaton Method

#### 3.1 Similarities and Differences between Phase Field Model and Cellular Automata Model

Compared with the PF model, although the simulation results of the CA model do not depend on the computer unit mesh structure, they will be affected by the mesh-induced anisotropy, so the accuracy is lower than the PF model. However, due to the high accuracy and the large amount of computation, the simulation time required of PF model is much higher than that of CA model. In addition, the PF model has limited computational range, while the simulation area of the CA model can reach the first level of casting. These advantages of CA model make it more suitable for simulating the formation of free dendrites or columnar dendrites, the deflection behavior in the flowing melt, and the columnar-to-equiaxed transition (CET) [6].

A melt pool formed during the LAM process of most alloy can reach several millimeters in size, so the workload is too large if adopting PF method for simulation. Furthermore, in recent years, the research on laser additive manufacturing iron-based alloy or titanium-based alloy has paid great attention to the columnar-to-equiaxed transition caused by undercooling. Therefore, CA method is more applicable to the prediction and exploration of alloy melt pool's solidification structure.

#### 3.2 Fundamental Theory of Cellular Automaton Model

The basic principle of the CA model is to divide the system into cells with the same size. When the CA model is used to simulate the solidification structure, the calculation of nucleation and growth are carried out on the finer mesh nodes by using the basic CA model. At present, the continuous nucleation model is usually adopted for the calculation of nucleation.  $\delta(\Delta T)$  is the undercooling which caused by a certain decrease of temperature in a time step. The density of new nucleation in the melt can be expressed as [7]:

$$\delta n_v = n_v [\Delta T + \delta(\Delta T)] - n_v(\Delta T) = \int_0^{\Delta T + \delta(\Delta T)} \frac{dn_v}{d(\Delta T')} d(\Delta T') \quad (6)$$

$$\frac{dn_v}{d(\Delta T)} = \frac{n_{\max}}{\sqrt{2\pi}\Delta T_\sigma} \exp\left[-\frac{1}{2}\left\{\frac{\Delta T - \Delta T_{mn}}{\Delta T_\sigma}\right\}^2\right] \quad (7)$$

where  $\Delta T_{mn}$  is the undercooling of average nucleation,  $\Delta T_\sigma$  is the standard deviation,  $n_{\max}$  is the maximum density of nucleation. After the nucleation, the schematic diagram of crystal growth in CA model as shown in Fig. 1.

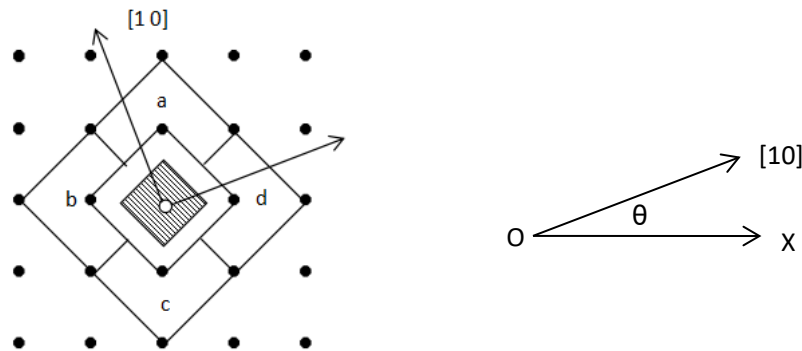


Fig. 1 Schematic diagram of crystal growth in CA model

As shown in Fig. 1,  $L$  is the distance between the adjacent CA mesh, the central shadow part is a nucleation node of the mesh unit, the radius of the grain is defined as the half diagonal length of the central shadow region. At a time,  $t_1$ , the square grain grown up on the nucleation node are exposed to four adjacent units of  $a$ ,  $b$ ,  $c$ ,  $d$ . The angle between the growth direction and the  $x$  axis is  $\theta$ , the

radius of crystal is  $L(t)=L(\cos\theta+|\sin\theta|)$ . Subsequently, the four unit nodes continue to grow up. At a time,  $t_2$ , grain growth is achieved by trapping eight nodes which are adjacent to  $a, b, c, d$ , and so on.

### 3.3 CA Simulation Method of Solidification Microstructure of Alloy Melt Pool

The low accuracy and the lack of comprehensiveness have hindered the CA model's application in the field of laser solid forming. According to the equation  $\lambda_1 \propto v^{-a} G^{-b}$ , where  $\lambda_1$  is the primary dendrite spacing,  $v$  is the rate of solidification,  $G$  is the temperature gradient, Yin et al. [3] only simulated the solidification information of the primary dendrite spacing. Northwestern Polytechnical University adopts adaptive mesh technology, and proposes a low anisotropic CA model. This model improves the rules of the cellular capture and interface curvature calculation, so it not only can simulate the whole microstructure of alloy melt pool, but also reflect the details of secondary dendrite spacing, the layer structure, the columnar-to-equiaxed transition and so on [8]:

The Solidification Technology Laboratory in Northwestern Polytechnical University uses the minimum neighbor solid-phase fraction method to reduce the anisotropy. First, the average solid fraction of the neighboring cells around a liquid cell is recorded as  $f_{S1}$ . The minimum solid fraction of a liquid cell captured is recorded as  $f_{S2}$ , and the proper value of  $f_{S2}$  can reduce the anisotropy of crystallographic orientations. Finally, if  $f_{S1} > f_{S2}$ , the liquid phase cell can be trapped into the interfacial cell.

The method of partial derivative of solid fraction is adopted to calculate the interfacial curvature, as shown in equation (8):

$$k = \frac{2 \frac{\partial f_s}{\partial x} \frac{\partial f_s}{\partial y} \frac{\partial^2 f_s}{\partial x \partial y} - (\frac{\partial f_s}{\partial y})^2 \frac{\partial^2 f_s}{\partial x^2} - (\frac{\partial f_s}{\partial x})^2 \frac{\partial^2 f_s}{\partial y^2}}{[(\frac{\partial f_s}{\partial x})^2 + (\frac{\partial f_s}{\partial y})^2]^{3/2}} \quad (8)$$

In order to improve the accuracy of calculation results, a partial derivative method which can be used to solve the equation is expressed as follows:

$$\begin{aligned} f_{s_{x,j+1/2,j+1/2}} &= \frac{1}{2dx} (f_{s_{i+1,j}} - f_{s_{i,j}} + f_{s_{i+1,j+1}} - f_{s_{i,j+1}}) \\ f_{s_{y,j+1/2,j+1/2}} &= \frac{1}{2dy} (f_{s_{i,j+1}} - f_{s_{i,j}} + f_{s_{i+1,j+1}} - f_{s_{i+1,j}}) \\ f_{s_{x,j,j}} &= \frac{1}{4} (f_{s_{x,j+1/2,j+1/2}} + f_{s_{x,j-1/2,j+1/2}} + f_{s_{x,j+1/2,j-1/2}} + f_{s_{x,j-1/2,j-1/2}}) \\ f_{s_{y,j,j}} &= \frac{1}{4} (f_{s_{y,j+1/2,j+1/2}} + f_{s_{y,j-1/2,j+1/2}} + f_{s_{y,j+1/2,j-1/2}} + f_{s_{y,j-1/2,j-1/2}}) \end{aligned} \quad (9)$$

## 4. The problems and Development Prospects

There are some limitations and problems in the current study:

- (1) Most simulations of LAM have neglected the process of powder addition.
- (2) The formation of alloy melt pool is affected not only by the temperature field, but also by the flow field and solute field. However, at present, few field coupled simulation studies are carried out at home and abroad, which leads to the lack of accuracy of the current numerical model.
- (3) With the development of solidification theory, the CA model is increasingly complex. Therefore, the existing solution method can not meet the demand of rapid and accurate calculations.

In conclusion, the development of simulating solidification microstructure must be based on the optimization algorithm and the increase of calculation speed. In addition, multi-condition and multi-field can be coupled to predict the evolution laws and characteristics of complex microstructure.

## 5. Acknowledgements

This work was financially supported by National Key R&D Program of China (2016YFB1100201), National Natural Science Foundation of Liaoning United fund (U1508213).

## References

- [1] H.M. Wang. *Acta Aeronautica et Astronautica Sinica*. 35 (2014) 2690-2698.
- [2] J.H. Li, A.Y. Xu, Q. Wang, M. Zhang. *Hot Working Technology*. 43 (2014) 16-19.
- [3] H. Yin, S.D. Felicelli. *Acta Materialia*. 58 (2010) 1455-1465.
- [4] D.J. Sun, J.C. Liu, Q.D. Li. *Chinese Journal of Lasers*. 40 (2013) 93-98.
- [5] V. Fallah, M. Amooezaei, N. Provatas, S.F. Corbin, A. Khajepour. *Acta Materialia*. 60 (2012) 1633-1646.
- [6] R. Chen, Q. Xu, B. Liu. *Journal of Materials Science & Technology*. 30 (2014) 1311-1320.
- [7] B.W. Shan, L. Wei, X. Lin, W.D. Huang. *Foundry*. 55 (2006) 439-443.
- [8] L. Wei, X. Lin, M. Wang, W.D. Huang. *Acta Physica Sinica*. 64 (2015) 348-355.