Phase field study of spacing evolution during wire and laser additive manufacturing under transient conditions

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Abstract. Understanding the dynamic evolution of primary dendritic spacing in the laser melt pool is significant from a technological viewpoint because primary spacing is one of the foremost parameters that control the final mechanical properties of additive manufactured products. In this work, a multi-scale computational framework that couples FEM and a developed quantitative phase field method is employed to simulate the evolution of microstructure and primary spacing of a nickel-based superalloy during wire and laser additive manufacturing (WLAM) solidification. Transient conditions in the laser melt pool are considered in which both temperature gradient $G$ and solidification speed $V_P$ are made time-dependent. Through the use of this model, the dendritic morphology, tip velocity and spacing evolution during the solidification are investigated to provide the relationship between the laser processing parameters and the final spacing. Moreover, we attempted to clarify the intrinsic mechanism of spacing adjustment under different laser processing parameters from a novel perspective. This work provides meaningful understanding of spacing evolution in nickel-based superalloy and demonstrates the potential of controlling the complex microstructure morphologies and final primary spacing during wire and laser additive manufacturing process.

1. Introduction

Metal-based additive manufacturing (AM), also known as three-dimensional (3D) printing, is a novel manufacturing technique across multiple industry fields, including the automotive, biomedical and aerospace industries [1, 2]. Wire and laser additive manufacturing (WLAM) is a new type of AM process in which large metallic materials can be fabricated layer by layer [3-5]. In this AM process, wire is fed at a constant rate into a laser beam and is melted onto a substrate or the previously deposited layer. After completion of one layer, the wire feeding–scanning–melting–solidification process is repeated until the whole component is built. Solidification in the laser melt pool controls the dendrite sizes, dendritic orientation, dendritic morphology, segregation of secondary elements and ultimately the properties of the product. Therefore, it is critical to investigate the solidification behaviour in the laser melt pool.

In the solidification environment generated by the laser additive manufacturing process, the microsegregation patterns and primary arm spacing are two primary components of columnar dendrites growth. These features have critical effects on both the mechanical properties of the as-built products and the subsequent heat treatment processes [6]. However, the primary arm spacing across the dendrites during laser additive manufacturing have not received enough attention yet. To improve the properties of the final product, a fundamental knowledge of the growth of dendritic morphologies during laser melt pool solidification is required.

To date, few studies have been done to simulate the dendritic morphologies developed in laser additive manufacturing processes using phase-field methods. In 2008, A Farzadi et al. [7] investigated the solidification conditions and dendritic morphology during the directional solidification in gas tungsten arc welding of Al–3wt%Cu alloy using the phase-field model. However, the simulated primary dendrite spacing was found not to be in a reasonable agreement with the predictions of the theoretical model proposed by Hunt et al [15]. In the study conducted by V. Fallah et al. [8], a thin-interface phase-
field model was coupled to a new heat transfer finite element model of the laser powder deposition process (during this process, a fiber laser was used to deposit the injected powder). The accuracy of the coupled model was validated by studying spacing evolution of Ti–Nb alloys. This work demonstrated the potential of simulating topologically complex microstructures present in laser additive manufacturing process. Using three modeling techniques - Finite element method, phase-field, and CALPHAD-based solidification models, Trevor Keller et al. [9] systematically investigated the microsegregation between dendrite arms, the primary arm spacings and the composition profiles during laser powder bed fusion (LPBF) process of IN625 alloys. However, the so-called steady-state solidification conditions throughout the entire process with constant temperature gradient and solidification velocity were used in all of the investigations above. This indicates that none of these studies has considered the variation in solidification conditions along the S/L interface within the solidifying melt. Although steady-state solidification is an important academic issue, it is far from representing the complex conditions really occur in the laser melt pool during WLAM process conducted in the current work. Therefore, understanding of the melt pool solidification behaviour under transient conditions in which both the pulling speed and thermal gradient are time-dependent variables is essential.

The objective of this paper is to perform numerical simulations, in two dimensions, of the microstructure evolution, and spacing evolution during wire and laser additive manufacturing of nickel-based superalloy GH3039 using the finite element method and phase-field model.

2. Model description

A double ellipsoidal volumetric heat source model is used to describe the laser melting process. To numerically solve the equations of three-dimensional heat transfer, a general FEM (finite element method) computer software, ANSYS 18.0, is utilized. In the present work, numerical results are presented for the case of a single-track laser deposition, however these can be translated to multilayer geometry by iterative solution over different layers. The thin interface 2D Karma phase-field model of alloy solidification [10] is used to investigate microstructure evolution in the laser melt pool. This model has been developed by Nikolas Provatas and co-workers [11]. Alloy solidification during WLAM process can be regarded as directional solidification which is assumed to be two-dimensional and with surface-tension anisotropy $\gamma$, moves in the $z$ direction at a time-dependent solidification velocity $V_P$ in an externally imposed time-dependent temperature gradient $G$. A phase-field parameter $\varphi$ is employed here, which takes the value $\varphi = 1$ (-1) in the solid (liquid). The complete set of the phase-field equations including crystalline anisotropy can be found in our previous work [12]. For the microscopic phase-field simulations, the diffuse interface parameters are chosen as $W = 0.27 \mu m$ and $dx = 0.8 W$, yielding $\lambda = 20.913$and $W / d_0 = 23.66$, which have been tested for convergence study. The dimensionless discretization time $dt = 0.004$. The GH3039 alloy (Nickel-based superalloy) is employed in this paper. Chemical composition (wt.%) of the selected GH3039 alloy is shown in Table 1. It should be noted that we have approximated the alloy GH3039 to be a binary alloy Ni-20.835 wt.% Cr. The thermophysical parameters of Ni-Cr binary alloy are as follows [13, 14]: the melting point of pure Ni $T_m = 1455$ K and the liquidus temperature $T_L = 1693$ K, equilibrium partition coefficient $k = 0.714$, slope of the liquid line $m = -2.1$ K/wt.%, liquid diffusion coefficient, $D_L = 2.0 \times 10^{-9}$ m$^2$/s and Solid diffusion coefficient, $D_S = 3.7 \times 10^{-13}$ m$^2$/s, Gibbs-Thomson coefficient $\Gamma = 2.0 \times 10^{-7}$ K/m, anisotropy $\varepsilon = 0.03$.

In this work, the FEM heat transfer model is used to simulate temperature distribution of the laser molten pool. The time-dependent temperature gradient and pulling velocity can be obtained from the FEM simulation results. Microstructure evolution during transient solidification will be simulated using the developed quantitative phase-field model. Following this, the multi-scale computational framework will be used to predict the spacing evolution of GH3039 alloy during WLAM process.
Table 1. Nominal chemical composition of the GH3039 alloy (wt.%).

| Element | Composition (wt.%) |
|---------|-------------------|
| Cr      | 20.835            |
| Mo      | 2.14              |
| Ti      | 0.62              |
| Nb      | 1.10              |
| Al      | 0.61              |
| Fe      | 1.09              |
| C       | 0.09              |
| Ni      | Bal.              |

Table 2. Conditions for the simulations of the laser melt pool.

| Parameter | $P$ (KW) | $V_s$ (mm/s) | h (mm) | $T_h - T_L$ (K) |
|-----------|----------|--------------|--------|-----------------|
| Case 1    | 2        | 10           | 2.8    | 1.5             | 1010             |
| Case 2    | 2        | 8            | 3.2    | 1.8             | 1100             |
| Case 3    | 2        | 6            | 3.6    | 2.1             | 1250             |
| Case 4    | 2        | 4            | 4.9    | 3.2             | 1360             |
| Case 5    | 1.5      | 10           | 2.3    | 1.2             | 950              |
| Case 6    | 2.5      | 10           | 3.9    | 2.1             | 1080             |
| Case 7    | 3        | 10           | 5.2    | 2.8             | 1200             |

Figure 1. (a) Schematic illustration of the experimental setup for WLAM process. (b) Solidification in the laser melt pool. (c) FEM simulation results of $G(t)$ and $V_P(t)$. (d) Time evolution of the cooling rates. In (c) and (d), a typical case of $P = 2$ KW, $V_s = 10$ mm/s was used.

3. Results and discussion

3.1. FEM simulations of the laser melt pool

Figure 1(a) shows the schematic illustration of the experimental setup and processing procedure during WLAM process. In Figure 1(b), the illustration of the solidification in the laser melt pool is presented, macro-scale morphology of the laser molten pool can be regarded as a quarter of ellipse, $V_s$ is the laser scan speed, $h$ and $b$ are depth and width of the laser molten pool respectively. The conditions for the FEM simulations of the laser melt pool are listed in Table 2, $T_h$ is the highest temperature of the melt pool. As shown in Figure 1(b), $V_P(t)$ increases rapidly from zero at the bottom of the laser melt pool to a larger value at the rear of the melt pool interface. We can calculate the time-dependent $G(t)$ and $V_P(t)$
under transient conditions in the laser melt pool [12]:

\[ V_P(t) = hV^2t / [V^2t^2 (h^2 - b^2) + b^4]^{1/2} \]

and

\[ G(t) = (T_h - T_L) / [V^2t^2 + h^2(1 - (V^2t^2 / b^2))]^{1/2} \].

Figure 1(c) and (d) shows the time evolution of simulated \( G(t) \), \( V_P(t) \) and the cooling rate under transient conditions. The cooling rate \( R \) is a significant variable in determining the microstructures in the laser melt pool which can be defined as: \( R = G(t) \times V_P(t) \). It is reasonable to conclude that compared to traditional steady-state conditions, this transient solidification conditions where the solidification speed and temperature gradient are both time-dependent values are closer to the real solidification condition in the laser melt pool.

3.2. Phase-field simulations of microstructure evolution

Understanding the evolution of microstructure morphology and interface velocity is critical for analysis of spacing evolution. Figure 2(a) shows simulated evolution of microstructure during the solidification of GH3039 alloy under Case 4 listed in Table 2. The interface morphologies transform into a relatively uniform cellular array (a3) through the stages of planar interface, rudiment of cells (a1) and dendrite submerging stage (a2). The interface dynamics and microstructure selection are determined by the instantaneous interface velocity. Figure 2(b) shows the dynamic evolution of interface velocity, where stage 1, 2, 3 and 4 are used to denote the planar growth stage, the initial competitive stage, submerging stage and short-term stable stage respectively. After the initial planar instability, the tip velocity increases sharply, and becomes even larger than the growth velocity. In stage 3, the tip velocity is still larger than the pulling speed though the tip velocity decreases with time. As shown in Figure 2(a2), if the lagged dendrite with small spacing cannot release its solute around the dendritic tip due to the interdendritic interactions, this lagged dendrite will be eliminated by its neighbours. This process is usually called cell/dendrite submerging [11]. In stage 4, the survived cellular tip velocity is almost equal to the pulling velocity, and so as its growth acceleration. The surviving cells keep the primary spacing uniform for certain time by lateral adjustment as shown in Figure 2(a3). Under transient growth conditions with time-dependent solidification velocity, dimensionless tip undercooling \( \Delta \) varies with time even after the initial transient stage as shown in Figure 2(c).

![Figure 2](image-url)

**Figure 2.** A typical simulation case of Case 4 in Table 2 (\( P = 2 \) KW, \( V_S = 4 \) mm/s). (a) Phase field simulation results of microstructure evolution. The color contrast shows the normalized concentration field \( ct = ck / c_\infty \), where \( c \) is the actual concentration field and \( c_\infty \) is the initial alloy concentration. (b) Time evolution of the tip velocity. (c) Time evolution of dimensionless tip undercooling under transient conditions.

3.3. Primary spacing evolution of the cellular dendrites
Boundary conditions will strongly affect numerical results from phase-field simulations, especially the primary spacing of the columnar dendrites [11]. Figure 3(a) shows the dependence of the average primary spacing on the system width under Case 4 and 5. Phase-field simulations of the spacing evolution for Case 1-4 were carried out using the system width of 550 μm. For Case 5-7, the system width is chosen as 400 μm. In this section, effects of the laser processing parameters on the final primary spacing are investigated. As depicted in Figure 3(b), when the laser scan speed ranges from 4 mm/s to 10 mm/s with the same laser power given by 2 KW, the primary spacing decreases with increasing the laser scan speed. In addition, when the same laser scan speed is given by 10 mm/s and the laser power ranges from 1.5 KW to 3 KW, the primary spacing increases with increasing the laser power as shown in Figure 4(a). In the following, we will try to investigate the intrinsic reason of spacing adjustment under different laser processing conditions.

First, effect of the initial spacing should be considered. Figure 3(c1) and (c2) show the variations of the crossover time from the planar morphology to cellular patterns and the initial spacing at the crossover point with different laser scan speeds. When the laser scan speed is increased, the crossover time decreases, while the average initial spacing remains stable. This indicates that the increasing scan speed could promote the initial instability while having limited effect on the initial spacing. The same conclusions could be obtained in Figure 4(b1) and (b2) when the laser scan speed is fixed and the laser power varies. In both cases, it is difficult to study the selection mechanism of final spacing through the initial spacing, the evolution process after planar instability need to be considered.

In section 3.2, Figure 2(b) shows the dynamic evolution of interface velocity under Case 4. It is noteworthy that although all cases presented in Table 2 exhibit similar qualitative behaviour for the time evolution of the interface velocity, the duration of stage 1, 2, 3 and 4 is quite different. As shown in Figure 2(b), the duration of the stage 3 is defined as \( t_3 \), the maximum value of the interface velocity at stage 2 and the minimum value of the interface velocity at stage 3 are defined as \( V_{\text{imax}} \) and \( V_{\text{imin}} \), respectively. As seen from Figure 3(d1), the values of \( t_3 \) and \( t_3/t_2 \) increase when the laser scan speed is decreased from 10 mm/s to 4 mm/s. This indicates that the role of the submerging stage (stage 3) is becoming more essential in the whole evolution process. And in Figure 4(c1), both \( t_3 \) and \( t_3/t_2 \) increase with the increase of the laser power, showing that the submerging stage occupies a more significant status. The microstructures evolve much faster in stage 2 than in other stages and the interface velocity reaches its maximum value at the end of stage 2. In the submerging stage, the interface velocity is decreased and a minimum value occurs at the end of this stage. Figure 3(d2) shows \( (V_{\text{imax}} - V_{\text{imin}})/V_{\text{imax}} \) as a function of the laser scan speed. This value increases with decreasing the laser scan speed, which indicates that the gap between the maximum and minimum is getting larger. While in Figure 4(c2), the value of \( (V_{\text{imax}} - V_{\text{imin}})/V_{\text{imax}} \) keeps nearly zero with increasing the laser power, indicating that the interface velocity is almost uniform in this stage. Let us turn to the primary spacing adjustment in stage 3. In the submerging stage, though the interface velocity decreased, the interface velocity is still larger than the solidification speed. The primary spacing is smaller than the lower limit of the allowable range in stage 4 (short-term stable stage), accordingly, the spacing will be enlarged by the submergence of the cells. In stage 4, the surviving cells keep the spacing uniform for certain time by lateral adjustment. Although the growth conditions vary with time, the average spacing keeps nearly constant in the late stage of stage 4. Therefore, it is reasonable to believe that the final primary spacing will get larger with increasing the duration of stage 3 which can be measured by \( t_3 \) and \( t_3/t_2 \). From the analysis above, when a fixed laser power is used, the smaller the laser scan speed (when the laser scan speed is fixed, the larger the laser power), the longer the duration of the submerging stage. Thus, resulting in larger final primary spacing within the scope of the present study. This conclusion is consistent with the results shown in Figure 3(b) and Figure 4(a), indicating that this criterion is effective in predicting the final primary spacing for different laser processing parameters.
Figure 3. (a) Simulated primary spacing vs. the system width. (b) Average final primary spacing vs. laser scan speed. (c1) The crossover time and (c2) the initial spacing at the crossover point from four different laser scan speeds. (d1) Variations of $t_3$ and $t_3/t_2$ with the laser scan speed. (d2) $(V_{\text{imax}} - V_{\text{imin}})/V_{\text{imax}}$ as a function of the laser scan speed. It should be noted that in all cases the same laser power is given by 2 KW.

Figure 4. (a) Final average primary spacing vs. laser power. (b1) The crossover time and (b2) the initial average spacing at the crossover point for different laser power. (c1) Variations of $t_3$ and $t_3/t_2$ with the laser power. (c2) Variations of $(V_{\text{imax}} - V_{\text{imin}})/V_{\text{imax}}$ with the laser power. It should be noted that in (a) – (c) the same laser scan speed is given by 10 mm/s. (d) Compareation of simulated primary spacing with the analytical models of Hunt and Lu [12] and Kurz and Fisher [13].

The comparison between the simulated and analytical mean primary spacing is illustrated in Figure 4(d), the simulated values are larger than the Hunt-Lu model and are slightly smaller than the Kurz and Fisher model [15, 16]. Although a completed quantitative agreement between the simulated primary
spacing and the two analytical models is difficult to obtain, the appropriate tendency and the similar values demonstrate that the phase-field model can be a powerful tool for quantitative simulation of spacing evolution under transient conditions.

4. Conclusion
In this work, primary spacing evolution during wire and laser additive manufacturing process of GH3039 alloy were studied using a developed multi-scale model. The transient condition which is distinctively different from the traditional steady-state condition was derived by making the solidification speed and temperature gradient both time-dependent variables. Effects of the laser processing parameters on the final primary spacing were investigated. Primary dendritic spacing predicted by this multi-scale model agrees well with the analytical model proposed by Hunt and Kurz. We attempted to clarify the intrinsic mechanism of spacing adjustment under different laser processing parameters from a novel perspective. Results revealed that the final primary spacing will get larger with increasing the duration of the submerging stage which can be measured by \( t_3 \) and \( t_3 / t_2 \). This criterion demonstrates the potential of predicting the final primary spacing under different solidification conditions present in wire and laser additive manufacturing and other relevant casting conditions.

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