Prediction of the microstructural grain evolution during selective laser melting by a cellular automata method

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Abstract. The mechanical properties of additively fabricated metallic parts are closely correlated with their microstructural texture. Knowledge about the grain evolution phenomena during the additive manufacturing process is of essential importance to accurately control the final structural material properties. In this work, a two-dimensional model based on the cellular automata method was developed to predict the grain evolution in the selective laser melting process. The effectiveness of this presented model is proven by comparing the simulated and reported results. The influence of process parameters, like the scanning strategy, laser power, and scanning speed, on the microstructural grain morphology, are numerically evaluated.

1. Introduction
Metallic powder-based additive manufacturing (AM) is of capability to fabricate near-net shape parts by melting metal powder in a layer-by-layer manner directly from 3D CAD model [1-3]. This technique provides promising potential and already successfully applied in the fields of aerospace, automotive, medical implant, etc. To fully satisfy its service requirement, the AM fabricated part should first process mechanical properties beyond a certain specification [1, 4]. The mechanical behavior of additively manufactured metallic part is predominant by its inherent solidified microstructure characteristics such as grain size, grain orientation, texture, and present phases [4].

The grain size of metallic material $d$ mathematically correlates with its yield strength $\sigma_y$ by the Hall-Petch equation

$$\sigma_y = \sigma_0 + \frac{k_y}{\sqrt{d}}$$  

(1)

where $\sigma_0$ is the stress constant for starting dislocation motion, $k_y$ is the constant material strengthening coefficient. This equation shows that the smaller the grain size, the higher the yield strength, and vice versa. The grain orientation significantly affects the directional nature of material mechanical properties. With uniform grain size and orientation in all three orthogonal planes, the material properties are generally isotropic. If grain orientation predominates in one of the planes, the additively printed material behaves highly anisotropic performance as reported in numerous works. Knowledge about the grain evolution of metallic material and the influencing factors during AM process benefits the selection of process parameters to achieve the desired mechanical properties for end-up use. While the experimental observation of this process is nearly impossible, computational modeling provides a time- and expense-efficient alternative for a thorough understanding of its underlying physical mechanism.
Various attempts are made to predict the material microstructures during AM. However, AM is a complicated process with rapid high power density input and repeated heating and cooling cycles. Quantitative prediction of additively manufactured microstructures requires combined efforts in solidification modeling spanning several lengths and time scales [5, 6]. Atomistic scale simulation is able to predict the solid-liquid interfacial phenomenon relevant to rapid solidification regimes [7-9], such as surface tension anisotropy, kinetic coefficient, and molecular dynamics of metallic alloys. At this scale, the Phase-field method is proven to be able to quantitatively simulate the detailed morphologies and dynamics of solidification microstructures compared with experimental observation [6]. However, obtaining a certain size microstructure from phase-field modeling for material performance prediction, for instance by the crystal plastic finite element method, is usually of very expensive computational cost. The Monte Carlo method offers an alternative approach for modeling microstructure evolution during AM. This method is capable of simulating both the rapid grain growth within the heat-affected zone surrounding the melt pool and the formation of elongated grains oriented along the temperature gradient. Although computational efficiency for qualitative feature prediction, simulation based on the Monte Carlo method is far from exploring the physics of granular solidification nucleation and growth and representing the physics properly within its simulation frameworks [5]. Cellular Automata (CA) [10, 11] method has a tradeoff between quantitative numerical accuracy and affordable computational cost for large domain size [12]. Cellular Automata based simulation utilizes a stochastic process for modeling grain nucleation and a deterministic process to model grain growth [13].

As a complicated physical process, the microstructure evolution of AM part is strongly affected by process parameters such as laser power, scanning speed, scanning strategy, hatch spacing, layer thickness, etc. Common variability in the microstructures is the grain types due to thermal gradient and solidification rate [14-16], texture driven by scan patterns [17-20], and deleterious phase formation [21,21] during cooling. The large-scale feature of microstructural grain such as texture in AM fabricated metallic parts influenced by the scan strategy gives rise to anisotropic mechanical properties. However, the majority of reported microstructure modeling by Phase-field [8,9], Monte-Carlo [23], and Cellular Automata [10, 11] focus on only the single bead melting process. The effects of repeated reheating and cooling cycles due to multiple beam scans and subsequent layer fabrication leading to grain coarsening are not included in these microstructure modeling of AM process. To develop a model incorporated the effect of scan patterns for microstructure prediction and understanding the influences of process parameter are thus essentially necessary.

In this presented work, we present a two-dimensional model based on cellular automata method for the prediction of microstructural grain evolution during additive manufacturing process. The morphology and statistical characteristic of predicted grain of AM manufactured IN718 by implemented model were compared with reported results. Once the model accuracy is proved, the influence of scanning strategy, laser power, and scanning speed, on the grain evolution were assessed.

2. Methodology
The algorithm of Cellular Automata method is capable to describe the evolution of a physical system on the spatial and temporal scale by applying deterministic and probabilistic transformation rules [24]. The computational domain is spatially divided into finite cells with assigned states. The status of a cell is characterized by four variables: (a) a grain number variable is used to distinguish the grains from others, (b) a state variable defines the cell state as solid, liquid, or interface, (c) an orientation variable represents the grain preferential growth orientation, and (d) a solid fraction variable is given to track the transition from liquid to solid-state. The interface cell distinguishes the current melt pool and boundaries of solidifying grains. The state of one cell correlates with its eight (first and second) nearest neighbors in the presented CA method according to transformation rules. If one of its neighbor cells is in solid-state, this cell is identified as a solid-liquid interface. At the beginning of the iteration, new nuclei populate at interface cells based on the nucleation law [25].
\[
\frac{\partial N}{\partial t} = -2\mu_f (\Delta T) \frac{\partial T}{\partial t} (1 - f_s)
\]

(2)

where \( N \) is the total quantity of nuclei, \( \Delta T \) is the thermal gradient divided by the total bulk undercooling, \( \frac{\partial T}{\partial t} \) is the cooling rate, \( \mu_f \) is the nucleation parameter, and \( f_s \) is the solid fraction. The nucleation model incorporates the effect of total undercooling and cooling rate. The nucleation probability of the cells located at the interface cell is calculated using (3) for every time step

\[
dP = \frac{\partial N}{N^i}
\]

(3)

where \( N^i \) is the total number of cells labeled as interface state. The state of the cell will transfer from liquid to solid if with a calculated probability greater than a randomly generated number between 0 and 1. The model thus becomes a deterministic function of a rounded probability variable. After nucleation of the new solid nucleus, the preferential direction of grain growth \( \theta_n \) is assigned based on the normal direction between the nucleated cell and the moving heat source. The driving force for grain growth relates to the thermal undercooling at the solid-liquid interface. The velocity of the solid-liquid interface is calculated using (4) [26]:

\[
V_n = \mu_k (\Delta T)
\]

(4)

where \( \mu_k \) is the interface kinetic coefficient, and \( \Delta T \) is the thermal undercooling:

\[
\Delta T = \left[ \Delta T_r - \bar{\Gamma} K(t_s) \right]
\]

(5)

where \( \Delta T_r \) is the thermal undercooling, \( \Gamma \) is the Gibbs Thomson coefficient, and \( \bar{K}(t_s) \) is the mean curvature which is described by [25] as:

\[
\bar{K} = \frac{1}{l_s^2} \left[ 1 - 2f_s + \sum_{i=1}^{N} f_s(i) \right]
\]

(6)

where \( l_s \) is the cell size and \( N \) equals 8, the total number of neighboring the first and second nearest cells of the considering one. The anisotropic grain texture is taken into consideration by introducing the crystal growth velocity \( V_n \) as a function of crystal preferred growth direction \( \theta_n \) as:

\[
V_n = V_h \left[ 1 + \delta_k \cos \left[ \frac{\theta - \theta_n}{4} \right] \right]
\]

(7)

where \( \delta_k \) is the degree of kinetic anisotropy and \( \theta \) is the angle between the horizontal direction and the normal of the solid-liquid interface. The angle \( \theta \) relates to the gradient of solid fraction at the solid-liquid interface. Once the velocity \( V_n \) is obtained, the change rate of the evolving solid fraction at the interface cell is calculated using (8):

\[
\Delta f_s = G \frac{V_n}{l_s^2} \Delta t
\]

(8)

where \( \Delta t \) is the time increment and \( G \) is a geometric factor related to its nearest 8 neighbors. \( G \) is calculated using (9) as described by [26]:

\[
G = 0.4 \left( \sum_{a=1}^{4} b_1^a + \frac{1}{\sqrt{2}} \sum_{a=1}^{4} b_2^a \right)
\]

(9)

where \( b_1 \) and \( b_2 \) represent first and second nearest neighbors respectively in a square grid. The geometric factor accounts for higher solidification rate for first nearest neighbors compared to second nearest neighbors. Once the fraction solid of a cell becomes 1, the cell state changes from interface to solid. The simulation terminates once all cells are assigned as solid-state. The constants used in the presented work are: lattice size \( l_s = 1 \mu m \), interface kinematic coefficient \( \delta_k = 2 \times 10^{-6} \), Gibbs Thomson coefficient \( \Gamma = 1.7 \times 10^{-5} \), degree of kinetic anisotropy \( \delta_k = 0.7 \), and nucleation parameter \( \mu_f = 10^3 \).
3. Simulation results

3.1 Powder bead melting simulation
Quantitative prediction of microstructure evolution relies on accurate thermal conditions, i.e., thermal gradient and undercooling rate. For demonstration, we perform modeling of computational fluid dynamics (CFD) of the SLM process. The detailed theory involved in CFD modeling is omitted as out of the interest of this work. The bead (layer thickness 30μm) is packing with Inconel 718 powder (average particle diameter 20μm). A CW fiber laser source (180Watts, spot size 54μm, and scanning speed 600mm/s) with a Gaussian energy distribution heat source is deposited at the points of powder-ray intersections. The hatch spacing between subsequent laser track is 105μm. The temperature contour during the melting is shown in figure 1a. As the heat source moves, the melt pool continues to solidify at its tail region. Figure 1b shows the predicted temperature history at point A in figure 1a during the selective laser melting process. Rapid heating and cooling of the interested point under the influence of the first laser heating is predicted. Due to the subsequent pass of the neighboring laser track, the temperature peaks again. The second temperature peak may generate the coarsening phenomenon of solidified grains.

![Figure 1](image.png)

**Figure 1.** (a) CFD simulation about powder bead melting process under laser heating and (b) temperature history of point A obtained from CFD simulation.

3.2 Effect of parameters on thermal condition and melt pool geometry
Scanning strategy can greatly affect the evolution of microstructural grain. Figure 2 shows four commonly used scan patterns in AM process. The angle is defined as the intersection angle between the scanning track and the positive direction of the y-axis. With different scanning strategies, laser power, scanning speed, prepositive simulations were performed to evaluate the influence of process parameters on the thermal conditions and the melt pool geometries, as shown in Table 1. Table 1 indicates that the scanning patterns 0º-0º and 0º-180º yield almost identical thermal conditions in cooling rate and thermal gradient, and exactly the same geometries of the melt pool. Although perpendicular in scanning track between two successive layers, the 45º-135º pattern has a much smaller predicted value in cooling rate and thermal gradient, and obviously larger size in melt pool compared with the 0º-90º pattern. The 45º-135º pattern is actually the same as the 0º-90º pattern by rotating 45 º. Therefore, the geometry of the melt pool under 0º-90º pattern is about √2 times of the melt pool with a 45º-135º pattern. With increasing scanning speed, the melt pool becomes smaller in size, while larger laser power leads to gradually increased geometry of melt pool.

3.3 Validation of presented modeling
Comparison between predicted microstructural grains over 0.5mm by 0.5mm and experimentally observation is performed to evaluate the effectiveness of this developed model [1] as shown in figure 3. The process parameters are the same as the powder bead melting simulation, with a 45º-135º scanning
pattern (same as the reported result in [1]). From the grain map (figure 3a), the $xy$ plane is characterized by equiaxial grains under giving process parameters, similar to the reported results. Multiple sub-grains were observed in larger grain, which indicates the appearance of low angle boundaries. The grain size is determined using the circle equivalence method and the grain orientation represents grain morphology. Figure 3e presents the grain morphology of the $xz$ plane, characterized by columnar grains. Statistical comparison in grain size and orientation between predicted and experimental observation is carried out. The results indicate that the overall grain morphology and developed texture of additively manufactured IN718 are successfully obtained based on implemented model.

![Figure 2](image)

**Figure 2.** Schematic of scanning strategy. (a) $0^\circ$-$0^\circ$ pattern; (b) $0^\circ$-180$^\circ$ pattern; (c) 45$^\circ$-135$^\circ$ pattern; (d) $0^\circ$-90$^\circ$ pattern.

**Table 1.** Predicted thermal conditions and melt pool geometry with different process parameters of SLM.

| Scanning Path Angle | Laser Power / W | Scanning Speed / (mm/s) | Cooling Rate / (K/s) | Thermal Gradient / (K/m) | Melt Pool Geometry |
|---------------------|-----------------|-------------------------|----------------------|--------------------------|--------------------|
|                     |                 |                         |                      |                          | Width / mm         |
| 0$^\circ$ | 0$^\circ$ | 180 | 600 | 453340.2 | 3064648 | 0.208 |
| 0$^\circ$ | 180$^\circ$ | 180 | 600 | 452435.2 | 3078682 | 0.208 |
| 45$^\circ$ | 135$^\circ$ | 180 | 600 | 475650.1 | 2977538 | 0.198 |
| 0$^\circ$ | 90$^\circ$ | 180 | 400 | 234515.7 | 2169499 | 0.274 |
| 0$^\circ$ | 90$^\circ$ | 180 | 600 | 453508.2 | 2875699 | 0.207 |
| 0$^\circ$ | 90$^\circ$ | 180 | 800 | 668169.4 | 3478753 | 0.178 |
| 0$^\circ$ | 90$^\circ$ | 240 | 600 | 289549.9 | 2317928 | 0.266 |
| 0$^\circ$ | 90$^\circ$ | 300 | 600 | 240657.3 | 2562901 | 0.329 |

### 3.4 Effect of scanning pattern

The movement of the laser heat source in specific scan patterns is essential to stimuli the grain evolution during AM process. With the same parameters in laser power, scanning speed, hatch spacing, and layer thickness, the microstructure grain morphology of AM IN718 parts manufactured by four different scanning patterns in figure 2 are predicted by the presented CA model and shown in figure 4. Significant differences in grain characteristics are revealed with respect to different planes and scan strategies. For the parts with $0^\circ$-$0^\circ$ and $0^\circ$-180$^\circ$ patterns, columnar grains are observed in the $xy$ plane tilted to the center of the melt pool following the laser track direction. The texture was formed due to the repeated laser tracks. The predicted grain morphology of $xy$ plane using $0^\circ$-90$^\circ$ and 45$^\circ$-135$^\circ$ cross patterns is similar to a checkboard with elongated grains within each square. The edge length of the square equals the hatch spacing of AM parameter as 105$\mu$m. The majority of columnar grain in $yz$ plane of $0^\circ$-$0^\circ$ and $0^\circ$-180$^\circ$ patterns are aligned in the direction around 10$^\circ$ with respect to the part building direction, while the grain orientation of parts using cross patterns almost is coincident with $z$ direction. In general, the scan patterns have limited influence on the average grain sizes in $xy$ plane of AM parts using four different patterns, varying between 41$\mu$m-50$\mu$m. The grain sizes in $xz$ and $yz$ planes with cross patterns are significantly larger than the $0^\circ$-$0^\circ$ and $0^\circ$-180$^\circ$ patterns.
Figure 3. EBSD analysis of SLM IN718 samples. (a) predicted and (b) experimental grain map in $xy$ plane [1], (c) grain size and (d) orientation in $xy$ plane, (e) predicted and (f) experimental grain map in $xz$ plane [1], (g) grain size and (h) orientation in $xz$ plane.

Figure 4. Predicted grain morphologies of AM IN718 samples with four different scan patterns. (a) predicted grain map using $0^\circ-0^\circ$, (b) $0^\circ-180^\circ$, (c) $45^\circ-135^\circ$ and (d) $0^\circ-90^\circ$ patterns, (e) grain size in $xy$, (f) $xz$, and (g) $yz$ plane, (h) average grain size, (i) grain orientation in $xy$, (j) $xz$, and (k) $yz$ plane.
3.5 Effect of laser power
The laser power also has a strong influence on the evolution of microstructure grain since the thermal conditions closely related to the input heat source. Figure 5 compares the predicted grain of AM IN718 parts with three different laser powers as 180W, 240W, and 300W. For the part fabricated with 180W laser power, the grain in xy plane most orient in the direction approximately 10º from the laser scanning direction. The orientation of grain in xy plane becomes more randomized when the laser power is set as 300W. The columnar grains in xz and yz planes, however, turn into coincident to the part building orientation with large laser power. The formation of unidirectionally oriented grains at high power using cross scan patterns is attributed to the following reasons: (1) lower cooling rate and thermal gradient induced lower nucleation rate, (2) grain coarsening during remelting of the previous layer, and (3) less grain competition due to the low number density of grains. With increasing laser power, the size of the predicted grain in all three planes becomes larger. Table 1 shows that the effect of high power in the implemented model is incorporated by reducing the cooling rate and thermal gradient.

![Figure 5](image_url)

**Figure 5.** Predicted grain morphologies of AM IN718 samples with different laser power. (a) predicted grain map with laser power 180W, (b) 240W, and (c) 300W, (d) grain size in xy, (e) xz, and (f) yz plane, (g) average grain size, (h) grain orientation in xy, (i) xz, and (j) yz plane.

3.6 Effect of scanning speed
The effect of scanning speed on the grain evolution of AM IN718 is also investigated. As shown in Table 1, faster scanning speed yields a much larger cooling rate and thermal gradient, and a smaller size in melt pool geometry. The trend of grain size and orientation characteristic in all three planes of AM part fabricated at increasing faster scanning speed is quite similar with the one manufactured under decreasing laser power. The reason is straightforward to understand. Due to faster scanning speed, a larger cooling rate, and thermal gradient would accelerate the nucleation rate of the interface cells. Also,
the remelting phenomenon of the previous layer caused by the subsequent layer fabrication is alleviated since the geometry of the melt pool is much smaller if with faster scanning speed. The grain coarsening effect becomes diminished.

Figure 6. Predicted grain morphologies of AM IN718 samples with different scanning speed. (a) predicted grain map with laser power 400mm/s, (b) 600mm/s, and (c) 800mm/s, (d) grain size in xy, (e) xz, and (f) yz plane, (g) average grain size, (h) grain orientation in xy, (i) xz, and (j) yz plane.

4. Conclusion
In this work, a two-dimensional model based on Cellular Automated method was developed to predict the microstructural grain evolution during the additive manufacturing process. The thermal conditions as undercooling rate, and thermal gradient, and the geometry of melt pool of AM IN718 parts are found closely related to its scan patterns, laser power, and scanning speed. The effectiveness of the presented model was proved as the characteristics of grain size, the orientation of predicted grain morphology well agrees with the reported observation. Using the developed model, the influences of different process parameters on the microstructure grain were assessed. Experimental validation is necessary to further optimize the developed CA model in the future.

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