Mesoscopic simulation of overlapping behavior in laser powder bed additive manufacturing

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Abstract
The prediction of the flow behavior of Metal micro-molten pool is prerequisite for high-quality Laser Powder Bed Fusion (L-PBF). In this study, mesoscopic scale numerical simulation modelling for L-PBF process was used to help understand the melting process of pure copper micro-melt pool. In this study, the orthogonal test was designed to study the influence of laser power, laser scanning velocity, hatching space on the flow behavior of molten pool and the overlapping rate of adjacent molten tracks. The results shows that laser scanning speed has the greatest influence on both the size and overlapping rate of the molten pool, and the overall trend was that the size of molten pool continues to increase as the volume energy density increases, and the maximum molten pool size was 243.6 \textmu m \times 110 \textmu m with volume energy density 370.037 J mm\textsuperscript{-3}, overlapping rate of adjacent molten tracks was 48.84\% with volume energy density 285.71 J/mm\textsuperscript{3}. The optimized pure copper laser process parameters were obtained: laser power 300 KW, laser scanning speed 500 mm/s, hatching space 0.07 mm, overlapping rate 48.84\%.

1. Introduction
Laser Powder Bed Fusion (L-PBF) is one of the most promising techniques in metal additive manufacturing. During L-PBF forming, the melting and solidification time of the micro-melting pool is less than 10\(^{-4}\) S, involving mass transfer, phase transformation and vaporization \cite{1, 2}. The mesoscopic scale simulation provided an effective method to study molten pool for L-PBF, from the laying of metal powder bed, the heating and melting of powder bed, the flow in the molten pool to the simulation of solidification forming \cite{3}. Compared with the macroscopic simulation, the mesoscopic scale simulation has higher resolution, which can better study the process of powder particle melting \cite{4-6}. In addition, mesoscopic-scale simulations can take into account the surface tension of the molten pool \cite{7}, the recoil pressure due to the evaporation of the molten pool, the Marangoni shear force, gravity, the thermal convection, radiation and heat conduction of the molten pool, the evolution of the molten pool and the mechanism of physical changes, and predict the defects such as pores and cracks caused by the melting of metal powder \cite{8, 9}.

Lee \textit{et al} \cite{10, 11} used open source discrete element software to consider particle size and distribution of powder, and single track and double tracks for L-PBF were established with evaporation and Marangoni flow of molten pool into account. The effects of laser power, velocity and powder particles on forming geometry and
babling were analyzed. Gurtler [12] used open source software OpenFOAM to achieve laser beam melting (Laser Beam Melting). With a simplified powder bed, regardless of the random distribution of the powder, the powder particles size was consistent, neatly arranged in the way of stacking. Gaussian bulk heat source was used for laser heat source. The influence of scanning distance and laser scanning speed on molten pool was analyzed. Zohdi [13] provided a systematic introduction to detailed material models and computational methods in additive manufacturing, including Basic Continuum Mechanics (CM), Discrete Element Method (DEM) and Smooth Particle Hydrodynamics (SPH) method [14], and pointed out a number of challenges, from the point of view of the end user of a simulation tool to be addressed in the development of computational approaches for additive manufacturing [15]. Yan et al. [16, 17] established Electron beam selective melting (E-BSM) by finite volume method, and the formation mechanism of defects such as spheroidization was analyzed by a single channel simulation. The s and z scan paths were simulated in the formation of multichannel tracks, which further clarified the forming mechanism and predicted potential defects. Xiang [18] used discrete element software to establish Ti₆Al₇V powder bed with random distribution of powder particles, Considering physical phenomena such as heat conduction, radiation, convection and evaporation, A VOF method was used to track the free liquid level, and the effect of Marangoni convection and recoil pressure on the morphology and flow of molten pool was studied. Dai et al. [19, 20] established the three-dimensional kinetic model of SLM forming W-Cu mixed powder by using the Fluent software. The temperature field and the force of W particles in the molten pool and the variation of the surrounding flow field were analyzed at different laser power and velocity. Pan [21–23] studied molten pool structure, velocity flow and temperature flow for pure copper by mesoscopic numerical model. Dai [24] investigated the effects of processing parameters on the thermal behavior during selective laser melting (SLM) of Ti-based composites by mesoscopic simulation.

Nowadays, there are few studies on SLM forming pure copper parts, which is easy to oxidize, with higher laser reflectivity and high thermal conductivity. XIA [25] explored the feasibility of fabricating pure copper parts by Selective Laser Melting by both experiment and mesoscopic numerical simulation. For pure copper, the overlapping rate can intuitively reflect the connection degree of the adjacent molten tracks, to obtain the optimized laser process parameters. Mesoscopic numerical simulation has been widely used in the field of metal additive manufacturing, but most focused on the optimization of laser process parameters, the temperature and velocity field of molten pool and the mechanism of defects. On the basis of previous research [21–23], this study focused on overlapping behavior research, two-passes laser scanning mesoscopic numerical simulation modelling was applied in this paper, and the molten pool structure and sizes of pure copper were studied. More importantly, the overlapping behavior of adjacent molten tracks, the velocity evolution and temperature evolution of typical positions after lapping were studied.

2. Material and method

2.1. Material properties
Air atomized pure copper powder is selected for L-PBF [23]. Of the powder material was 15–53 μm. Table 1 showed pure copper powder properties and detailed data are provided in [25].

2.2. Model of L-PBF
Figure 1 showed the finite element model of L-PBF, mainly including laser beam substrate and pure copper metal powder. EDEM was used to complete the particle size and distribution of metal powder (particle size 15 μm – 53 μm, random distribution). On this basis, the metal powder and substrate model were imported into Flow 3D.

In order to study the overlapping rate of adjacent tracks, two-passes laser scanning was applied. The size between two-pass laser scanning molten track was hatching space, and the specific scanning direction was shown in figure 1.

In this work, details of the computational method was listed as below: Hexahedron was chosen as type of element with the mesh size 5 μm, free surface was chosen as interface tracking method, Incompressible flow mode was chosen as flow mode. The simulation for each extreme takes about 10 h with the the technical specification of the computer as below: Intel(R) Core(TM) i7-8750H CPU @ 2.20 GHz 2.21 GHz, RAM 8.00 GB.

In addition, basic on previous research [21, 23], moving Gaussian surface heat source was chosen as heat source model. The metal powder layer geometry is initialized using the results from DEM simulation, and the melting and solidification process of metal powder after laser irradiation adopts computational fluid dynamics (CFD) Simulation.

Besides, heat transfer forms mainly includes heat conduction, heat convection and heat radiation during L-PBF process: the heat convection and heat radiation models of the material surface and the surrounding environment are as below [25]:

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**Table 1: Pure Copper Powder Properties**

| Property          | Value          |
|-------------------|----------------|
| Particle Size     | 15–53 μm       |
| Material          | Pure Copper    |

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Where, $s$ is the Stephen-Boltzmann constant, $W/Km^2$, $h$ is the convection exchange coefficient ($W/Km^2$); $n$ is the surface normal direction.

### 2.3. Orthogonal test method

The authors had carried out some work on the preparation of pure copper by L-PBF \cite{23}. On this basis, in order to determine the influence of laser power, laser scanning velocity, hatching space on the flow behavior of molten pool and the overlapping rate of adjacent molten tracks, the orthogonal test of 3 factors 2 level was designed: laser power (300 KW, 500 KW), laser scanning velocity (500 mm s$^{-1}$, 2500 mm s$^{-1}$), hatching space (0.07 mm, 0.09 mm), as shown in table 2.

In this paper, the evaluation indexes of orthogonal test numerical simulation were as follows: (1) the size of the micro-molten pool and (2) the overlapping rate of the adjacent molten tracks.

### 3. Results and discussion

#### 3.1. Molten pool structure

Taking the forming experiment of scheme no. 1 as the research object. Figure 2 showed the morphology of molten pool. The front end of the molten pool was concave, with the overall size 140 $\mu$m $\times$ 150 $\mu$m $\times$ 50 $\mu$m. It should be noted that the concave depth in the upper surface center of the molten pool was small, which was mainly due to the low laser scanning speed (500 mm s$^{-1}$) with a small impact on the molten metal.
Figure 3 showed the morphology of molten track of scheme no. 1. The surface of molten track was more flat after solidification, no sharp unevenness. Because of the high volume energy density, the width of the molten track reached 180 um. In addition, compared with AlCu5MnCdVA alloy [21], the depth of the heat affected zone (HAZ) reached 100 um, much higher than AlCu5MnCdVA alloy 20 um. The reasons can be summed up as the extremely high thermal conductivity: thermal conductivity for pure copper was 377 W/(m·K), which was almost 3.3 times of AlCu5MnCdVA alloy (113 W/(m·K)).

Figure 4 showed the morphology and solid fraction of scheme no. 1’s single pass molten track for pure copper. Colors represented solid fraction, where red represented liquid, blue represented solid, and the rest represented solid-liquid coexistence. As shown in figure 4(b), the two sides of the tail in molten pool solidified first, and the internal solidification was slightly slower.
3.2. Molten pool size

3.2.1. Molten pool size evolution law

Laser parameters (laser power, laser scanning velocity, hatching space, layer thickness) play a role in determining the size of the pool. In this paper, volume energy density is selected to comprehensive characterization of laser process parameters.

\[ E = \frac{P}{V \cdot h \cdot t} \]

Where, \( E \) is volume energy density, \( P \) is laser power, \( V \) is the Laser scanning velocity, \( h \) is hatching space, and \( t \) is layer thickness.

In this paper, volume energy densities for the four experiments are 285.71 J/mm\(^3\), 95.23 J/mm\(^3\), 44.44 J/mm\(^3\), 370.037 J/mm\(^3\), respectively.

Figure 5 showed the size of molten pool for the orthogonal test Schemes NO.1–4. The overall trend is that the size of molten pool continues to increase as the volume energy density increases.

3.2.2. Orthogonal test results and analysis

To determine the influence of laser power, laser scanning velocity, hatching space on the size of the micro-molten pool, the size of the micro-molten pool (mm\(^2\)) was set as the evaluation indexes of orthogonal test numerical simulation. Table 3 showed the results of extreme analysis for molten pool size.

As shown in table 3, laser scanning speed has the greatest influence on the sizes of molten pool, followed by laser power and hatching space.
3.3. Overlapping structure of adjacent molten tracks

For the same layer, the molten metal was connected by adjacent molten tracks. Therefore, the structure of adjacent tracks is very important for metal connection. In this paper, the overlapping rate is introduced to indicate the connection state:

\[
A = \frac{L_C}{L_1 + L_2 - L_C} \times 100\%
\]

Where, \(L_C\) was the length of superposition area for adjacent molten tracks, \(L_1\) was the length of the first-pass molten pool, \(L_2\) was length of first-pass molten pool.

As shown figure 6, there are three typical lap sates: ① the overlapping rate is too low, and the adjacent melt tracks cannot be connected to each other, which directly causes the metal to be unable to connect after solidification, and the strength decreases sharply. In addition, metal powder among between molten tracks cannot be completely melted, resulting in balling and pores defects; ② the overlapping rate is ideal. After the edges of the adjacent melt tracks are in contact, the edges remelted, which helps to strengthen the connection strength of the adjacent tracks. On the other hand, the originally concave edges are connected to each other, and the surface roughness is reduced, surface flatness is improved; ③ the overlapping rate is too large, which leads to the complete remelting of the previous molten track or the solid phase transformation at high temperature again, resulting in internal phases changing or coarse grains.

3.3.1. Overlapping structure

Figure 7 showed the schematic diagram of the lap morphology of adjacent molten track, which was mainly divided into four zones: ① superposition area of molten pools; ② superposition area of First-pass molten pool.
and second-pass HAZ; ③ superposition area of First-pass HAZ and second-pass molten pool; ④ superposition area of First-pass HAZ and second-pass HAZ.

Taking the forming experiment of scheme no. 1 as the research object. Figure 8 showed the structure of molten pools in two passes. Colors represents the solid fraction: red was liquid, blue was solid, the rest of the colors represented solid-liquid coexistence. Figure 8(a) showed the molten pool for the first-pass laser scanning. Because the laser beam radius was about 70 μm, the overall size for molten was 176.4 μm × 64 μm. In the process of molten pool forming, solid-liquid coexistence area is small, about 10 um thick. Figure 8(b) showed
Figure 9. Overlapping rate of adjacent molten tracks for four schemes.

| Scheme | Volume energy density (J/mm²) | Overlapping rate (°) |
|--------|-------------------------------|---------------------|
| 1      | 285.71                        | 48.84               |
| 2      | 95.23                         | 23.53               |
| 3      | 44.44                         | 0                   |
| 4      | 370.37                        | Forming failed      |

Figure 10. Overlapping results of adjacent molten tracks: (a) scheme no. 1; (b) scheme no. 2; (c) scheme no. 3; (d) scheme no. 4.
the adjacent molten pool for the second-pass laser scanning, overall size 210 \( \mu m \times 88 \mu m \). Figure 8(c) showed overlapping structure of molten pools: The overlapping length reached 126 \( \mu m \), which was an ideal state for adjacent molten tracks connection 4.

3.3.2. Overlapping rate
Due to the high thermal conductivity and low laser absorption, forming pure copper requires higher laser volume energy density than SS316L [25]. This paper designed orthogonal test to study the relationship between laser power, laser scanning speed and scanning spacing and lap rate.

Figure 9 showed a overlapping rate of adjacent molten tracks for four schemes: 48.84%, 23.53%, 0% and forming failed, respectively.

Therefore, the adjacent tracks connection of scheme no. 1 was ideal, and the overlapping rate was 48.84%. As shown in figure 10(a), the surface of the adjacent tracks was smooth, straight line state, and the surface flatness ensured both the uniformity of the next metal powder and surface roughness of solidified metal.

Figure 10(b) showed the adjacent tracks connection of scheme no. 2. The overlapping rate was 23.53%. Due to the low volume energy density (95.23 J mm\(^{-3}\)), the size of the molten pool decreased. More importantly, the surface was wavy and the surface roughness was reduced microscopically, which led to the uneven powder laying of the next metal powder and seriously affect the forming quality [24, 26, 27].

Figure 10(c) showed the adjacent tracks connection of scheme no. 3. It was obvious that the size of the molten pool was reduced due to the low linear energy density (44.44 J/mm\(^3\)). On the other hand, because the hatching space was large (0.09 mm), and the adjacent tracks could not be connected to each other and overlapping rate was 0%; the metal powder between adjacent molten tracks could not melt completely, and spheroidization and pores defects appeared.
Figure 10(d) showed the molten pool of scheme no. 4. Due to the excessive volume energy density (370.37 J mm$^{-3}$), the local temperature was as high as 4289 K (Boiling temperature was 2799 K), resulting in boiling, vaporization and spatter. Finally, the metal solution failure, cannot continue to calculate, and forming failed.

Figure 11 showed the overlapping morphology of scheme no. 1 for both experimental printing and numerical Simulation, and overlapping length was 110 um, 126 um respectively. Considering that the molten pools structure was unstable in the printing process and has certain fluctuations, the simulation results and experiments have high reference value [28].

3.3.3. Orthogonal test results and analysis
To determine the influence of laser power, laser scanning velocity, hatching space on the overlapping rate of the adjacent molten tracks, orthogonal test results were listed as below:

The evaluation indexes of orthogonal test numerical simulation was the overlapping rate of the adjacent molten tracks (%). Considering that scheme no. 4 failed to forming, the overlapping rate was set to 80%.

As shown in table 4, laser scanning speed had the greatest influence on the sizes of molten pool, followed by laser power and hatching space.

By comparing table 3 with table 4, the laser scanning speed has the greatest influence on both the size and overlapping rate of the molten pool, and the specific mechanism will be the focus of our later research.

3.4. Temperature evolution law for adjacent molten tracks
To study the internal temperature variation of the first-pass molten pool in the forming process of adjacent molten track, the center point of the first-pass molten pool was chosen as the study object, as shown in figure 12.

Figure 13 showed the temperature evolution law for two-pass laser scanning for the picked point. As shown in figure 9, Point A was the starting of laser scanning, and the temperature rose sharply to Point B (2680.0 K). Then laser beam moved away and temperature began to drop to Point C (1357.77 K): The temperature’s rising and dropping velocities reached an astonishing $2.7 \times 10^7$ K S$^{-1}$, $1.2 \times 10^7$ K S$^{-1}$, respectively. This was largely attributable to the high thermal conductivity: thermal conductivity for pure copper was 377 W/(mK), which was almost 23.3 times of SS 316L (16.2 W/(mK)).

From Point C to Point D, metal was in solidification stage, and the solidification time was about 0.0019 S. Therefore, the solidification in L-PBF was very fast and the grain size was too late to grow, so it can be predicted that the internal grain size was small, which was one of the advantages of L-PBF process. At the same time, because the gradient of temperature change was too large, it was easy to produce internal stress, which was a problem that L-PBF expected to solve [29, 30].
One interesting finding was that the metal powder undergone twice melting and solidification processes, as shown in the figure: Point C to Point D, which was the first-pass laser scanning; Point F to Point D, which was the second melting and solidification, attributed to the laser scanning of adjacent molten tracks [31, 32].

3.5. Velocity evolution law for adjacent molten tracks
Figure 14 showed the velocity evolution law for two-pass laser scanning of the picked point in the center of molten pool.

For x-direction (laser scanning direction), the velocity of the molten metal was mostly in the -x direction, which showed that molten metal flowed back during the formation of the molten track and maximum velocity reached $-1.3 \text{ m s}^{-1}$. After first-pass solidification, the solidified metal remelted again during the second-pass forming of the adjacent molten track, and liquid metal flowed back again in the x-direction with a maximum flow velocity of $-1.0 \text{ m s}^{-1}$.

For y-direction, the velocity of the molten metal was random fluctuation at the first-pass laser scanning, with the maximum velocity $0.8 \text{ m s}^{-1}$. An interesting phenomenon was the remelt metal flow velocity in the Y direction reached $1.5 \text{ m s}^{-1}$, almost 2 times than the first-pass $0.8 \text{ m s}^{-1}$: due to the double impact of the laser and the molten metal in the adjacent molten, the molten metal of the first pass flowed along y-direction faster [33].

4. Conclusions
By using mesoscopic numerical modelling, the molten pool structure of pure copper fabricate by L-PBF was obtained intuitively, including size and surface morphology. Moreover, the overlapping states of the adjacent
molten tracks for two-pass laser scanning showed a different structure, and the optimized pure copper laser process parameters were obtained: laser power 300 KW, laser scanning speed 500 mm/s, hatching space 0.07 mm, overlapping rate 48.84%, and the surfaces of the connected molten tracks was flat. Moreover, due to the high thermal conductivity of pure copper, HAZ area of the molten tracks was larger: the width and depth reached 100 um, 180 um, respectively.

Because of the overlap of the adjacent tracks edges, the velocity and temperature field were redistributed. Unfortunately, the laser process parameters used in the two-pass adjacent molten tracks were the same in this paper. But the velocity and temperature field internal could be controlled by controlling the temperature and velocity field by adjusting second-pass laser process parameters, which will be the focus of our next research.

**Data availability statement**

The data that support the findings of this study are available upon reasonable request from the authors.

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**Conflicts of interest**

The authors declare no conflict of interest.

**Availability of data and material**

Some or all data, models, or code generated or used during the study are available from the corresponding author by request.

**Code availability**

Not applicable.

**Ethics approval**

Not applicable.

**Consent to participate**

Not applicable.

**Consent for publication**

We consent to publish it in the journal Materials research express.

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