### A numerical investigation on the physical mechanisms of single track defects in selective laser melting

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A Numerical Investigation on the Physical Mechanisms of Single Track Defects in Selective Laser Melting

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Abstract

A three-dimensional high-fidelity model was developed to simulate the single track formation of stainless steel 316L during selective laser melting. Different laser powers and scanning speeds were adopted to perform the numerical simulations, revealing the underlying physics of porosity development during the melting and solidification process. Our studies suggest the importance of surface tension and recoil pressure in creating two types of porosities: near-spherical and irregular-shaped porosities. With excessive energy intensity, the predominant recoil pressure is liable to create a deep moving keyhole, resulting in entrapped gas bubbles with near-spherical geometries underneath the solidified track. Additionally, wetting behaviour between melted powders and the substrate below is proved to be significant in eliminating interlayer porosities with irregular configurations. A low energy intensity is possibly inadequate to melt the substrate below, suppressing the wetting behaviour and giving rise to the formation of interlayer defects. Furthermore, our multilayer simulations prove that the surface roughness of previously solidified layer plays a critical role in affecting the local thickness of next powder layer. The fluctuation of local powder thickness is probably associated with the formation of interlayer defects, as the energy intensity maybe not strong enough to penetrate a locally thicker powder layer.

Keywords:
Heat transfer; Computational fluid dynamics; Selective laser melting; Stainless steel; Porosity; Wetting

1. Introduction

Selective laser melting (SLM), with the advantages of fabricating freeform geometries and manipulating material microstructures, has been hailed as one of the most promising manufacturing technologies. The basic working principle of SLM is to selectively scan a layer of metal powders deposited on the baseplate by applying a focused laser beam directed by 3D CAD data. Upon absorption of the laser irradiation, the scanned powders are melted and then quickly solidifies, giving rise to the formation of a single track. The as-fabricated samples are then produced by repeating such process via a layer-by-layer manner.

Numerous studies have been carried out to establish the correlations between processing conditions and properties of SLM-processed materials, including residual stress [1], crack [2], microstructure [3, 4], mechanical properties [5] and porosity [6, 7]. Among these concerns, porosities are considered as a critical factor affecting the performance of as-built parts, as these internal defects can degrade the fatigue and mechanical properties [8]. Therefore, understanding how porosities are generated during SLM is of crucial importance to eliminate such flaws. Many previous experiments have been devoted to investigate the porosities within SLM-fabricated samples. Aboulkair et al. [9] proposed the required process maps to achieve high density parts of AlSi10Mg alloy. Their work demonstrated the correlations between the laser scanning speeds and the types of porosities. Spherically shaped porosities are formed with low scanning speeds, whereas large and irregularly shaped porosities are found with high scanning velocities. Garibaldi et al. [10] and Kaspeovich et al. [11] reported similar observations in high-silicon steel and TiAl6V4 alloy. Specimens fabricated with low energy inputs are characterized with irregularly shaped porosities, while bubble-like defects appear in
samples processed with high energy intensities. In comparison, medium energy densities are found to be appropriate to achieve defect-free samples.

Nevertheless, how porosities are created and how do they span over several layers during SLM are still open for discussion. Previous studies suspected different and even conflicting mechanisms of the porosity development (especially spherical porosities) in SLM-processed samples. Gong et al. [12] assumed that the formation of spherical porosities is attributed to spherical pits on the top surface, since the recoating blade scraps the particles solidified from the ejected molten materials. Qiu et al. [3] observed open pores on the top surfaces of the laser-processed TiAl6V4 samples, and claimed that near spherical porosities are due to incomplete re-melting of some localised surface areas of the previous layer and to the insufficient feeding of molten materials to these localised sites. King et al. [13] argued that spherical porosities are associated with the entrapped gas bubbles induced by keyhole mode melting. On the other hand, irregularly shaped defects are typically formed at the interlayer boundaries between two adjacent layers, and are believed to result from lack of fusion [14]. With the application of micro computed tomography (CT) techniques, Zhou et al. [15] observed single layer and multi-layers defects with irregular morphology. They proposed that the surface roughness of the prior layer would act as a perturbation source that intensifies the subsequent melt pool instabilities, thereby creating an even rougher surface. Such vicious circle can lead to the melt track discontinuities and structural defects in SLM-fabricated specimens.

With the complex physical phenomena at microsecond and micrometer scales, it is challenging to monitor the SLM process by experiments. An attractive alternative to reveal the physical mechanisms of SLM defects is through predictive numerical simulation [16]. Korner et al. [17] employed lattice Boltzmann method (LBM) to simulate the electron beam melting (EBM) process in 2D, including single layer and layer upon layer consolidation. Their results emphasized the importance of local powder arrangement on the undesirable balling effects.
However, the validity of LBM model is questioned due to the omission of the third dimension, as a real SLM process is asymmetric and inherently complex in three directions. Through computational fluid dynamics (CFD), Gürtler et al. [18] firstly reported a 3D mesoscopic model to examine the melting and solidification behaviours during SLM, which provides physical realism and qualitative agreements with experiments. Khairallah et al. [19, 20] used ALE3D code to analyse single melt tracks and discuss the physical mechanisms evolved during laser scanning. The simulation results demonstrated the dominant effects of surface tension, Marangoni force and recoil pressure in L-PBF manufacturing. They clarified that the coalescence of melted powders is primarily attributed to surface tension, whereas recoil vapor pressure can result in a depression site near the beam spot. Qiu et al. [6] predicted the fluid flow of regularly packed powders during SLM process, and proposed that increased scanning speed or powder layer thickness would trigger the splashing of molten materials and instability of scanned tracks. Similarly, Panwisawas et al. [21] noticed that the increment of layer thickness leads to the irregularity of scanned tracks. Lee et al. [22] demonstrated the effects of powder size and pack density on the geometry of scanned track. The surface roughness is found to be reduced with smaller powders, and high packing density is beneficial to eliminate the balling defects. The simulation study by Yan et al. [23] revealed the significance of powder size distribution and powder layer thickness in determining the nonuniformity of the scanned tracks. Their simulation of multiple tracks also suggested that the elimination of defects requires a hatch spacing smaller than the width of the fused zone.

The elimination of structural defects is one of the ultimate objectives of SLM. A clear understanding of the porosity formation mechanisms is thus a premise to achieve parts with high density. Previous PBF simulations were mostly focused on the low input energy regime. The formation of interlayer porosities and balling defects could be observed and the related physics have been discussed. By performing numerical investigations, the present study aims
to elucidate the physical origins of porosity development in both high and low energy regime. The multi-layer simulations can further explain the accumulation of porosities during the layer-by-layer fabrication. Single track simulations are presented to analyse the porosities formed in SLM stainless steel 316L (SS316L) alloy in relation to the processing parameters. The simulation findings exhibit consistency with previous experimental observations.

2. Modelling approaches

By using DEM and CFD, a 3D powder-scale model with high fidelity was developed to simulate the SLM process. Such mesoscopic model requires fine mesh grid size to resolve individual powder particles. Due to the high computational cost, the current study was limited to identify single track formation and the in-situ porosities within the consolidated materials. Despite the small computational domain considered, this study still sheds light on the mechanisms for porosity developments. Details of the model are discussed as follows.

2.1. DEM simulation of powder bed

An open source DEM code LIGGGHTS® (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations) [24] was adopted to model the random packing of SS316L particles laid on the solid substrate. Following the size distribution in ref [25] , the metal powders in this work are approximated as solid spheres with a mean diameter of 27 µm and a half maximum width of 10 µm.

Based on Newton’s second law of motion, morphology of the powder bed was achieved by calculating the trajectories of spherical particles. A cloud of metal powders was firstly created right above a cubic box. Due to gravitational and contact forces, these released powders freely deposited into the box and formed a powder bed. A recoating blade was then applied to spread a 50 µm high layer of metal particles, which is similar to the procedures reported in ref [26]. Finally, the sizes and positions of individual particles were extracted from the DEM results.
The DEM data was subsequently imported into the CFD model to determine the initial configuration of the powders laid on the substrate.

2.2. CFD simulation of heat transfer and melt flow dynamics

Based on an open source code OpenFOAM® (Open Field Operation and Manipulation) [27], a CFD model was developed to investigate the complex physical phenomena during additive manufacturing (AM) processing. A simplified ray tracing energy source with Gaussian distribution was implemented to represent the interactions between the powder bed and the applied laser beam. Various factors governing the flow kinetics, such as surface tension, Marangoni shear stress and recoil vapor pressure were incorporated in the CFD model. Several assumptions were made to simplify the simulation model: (1) The fluid flow in melt pool is Newtonian and laminar; (2) the thermophysical properties of SS316L are functions of temperature only; (3) plasma effect in SLM process is ignored. Following these assumptions, volume of fluid (VOF) and Navier-Stokes equations were solved to simulate the thermal fluid flow during AM. The VOF method [28] was employed to capture the dynamic geometry of the free surface (gas/metal interface). The volume fraction of metallic phase satisfies the following conservation equation:

\[
\frac{\partial (\bar{\rho} \alpha_i)}{\partial t} + \nabla \cdot (\bar{\rho} \overline{u}\alpha_i) = 0
\]

(1)

where \( \overline{u} \) is the flow velocity, \( t \) is time, \( \bar{\rho} \) is the volume-averaged density, \( \alpha_i \) is the volume fraction of metallic phase (\( 0 \leq \alpha_i \leq 1 \)). \( \alpha_i = 1 \) indicates a cell completely occupied by the metallic phase, and \( \alpha_i = 0 \) corresponds to a gaseous cell where no metal is present. Additionally, any material property of mixture \( \phi \) was computed based on the weighting/volume-averaged function, which can be defined as
\[ \bar{\phi} = \alpha \phi_{metal} + (1 - \alpha) \phi_{gas} \]  

For instance, the mixture density was calculated by \( \bar{\rho} = \alpha \rho_{metal} + (1 - \alpha) \rho_{gas} \). Moreover, a temperature dependent function \( \gamma \) is expressed as \[2\]

\[
\gamma = \begin{cases} 
0 & T < T_s \\
\frac{T - T_s}{T_i - T_s} & T_s \leq T \leq T_i \\
1 & T > T_i 
\end{cases}
\]  

where \( T_i \) and \( T_f \) are solidus and liquids temperature of SS316L, respectively. \( T \) is the temperature field of the computation domain. Accordingly, the volume fraction of solid metal \( f_s \) and liquid metal \( f_l \) are \( \alpha (1 - \gamma) \) and \( \alpha \gamma \), respectively. The material properties of SS316L \( \phi_{metal} \) can be described by

\[
\phi_{metal} = (1 - \gamma) \phi_s + \gamma \phi_l
\]  

where \( \phi_s \) and \( \phi_l \) represent the material properties of solid and liquid metal, respectively.

The mass conservation equation is considered as

\[
\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u}) = 0
\]  

The momentum equation is given by \[21\]

\[
\frac{\partial (\bar{\rho} \bar{u})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{u}) = -\nabla P + \bar{\rho} \bar{g} + \nabla \cdot (\bar{\mu} \nabla \bar{u}) + \bar{f}_{damp} + \bar{f}_{st} + \bar{f}_M + \bar{P}_r
\]  

where \( P \) is the pressure, \( \bar{g} \) is the gravity acceleration, \( \bar{\mu} \) is the dynamic viscosity. \( \bar{f}_{damp} \) is a damping force term associated with the energy dissipation in the mushy zone, and is described as \[21\]
\[ f_{\text{damp}} = -K_i \frac{(1-\gamma)^2}{(\gamma^3 + C_K)} \ddot{u} \] (7)

where \( K_i \) is the permeability coefficient, \( C_K \) is a small constant to avoid division by zero. The surface tension force \( f_{st}^- \) is written as [30]

\[ f_{st}^- = \sigma \kappa \bar{n} \frac{2\rho}{\rho_{\text{metal}} + \rho_{\text{gas}}} \] (8)

where \( \sigma \) is the surface tension coefficient of SS316L, \( \bar{n} \) is the unit normal vector at metal/gas interface, \( \kappa \) is the curvature of metal/gas interface. The term \( |\nabla \alpha| \) was adopted to transform an interfacial force per unit area into a volumetric surface force [30]. The multiplier term \( \frac{2\rho}{\rho_{\text{metal}} + \rho_{\text{gas}}} \) redistributes the interfacial forces toward the heavier phase (metal) [30], thereby improving the numerical stability of the model. The unit normal vector and the curvature of metal/gas interface can be expressed as

\[ \bar{n} = \frac{\nabla \alpha}{|\nabla \alpha|} \quad \text{and} \quad \kappa = -\nabla \cdot \bar{n} \] (9)

The Marangoni shear force \( f_{M}^- \) is given by [30]

\[ f_{M}^- = \frac{d\sigma}{dT} \left[ \nabla T - (\bar{n} \cdot \nabla T) \bar{n} \right] |\nabla \alpha| \frac{2\rho}{\rho_{\text{metal}} + \rho_{\text{gas}}} \] (11)

where \( \frac{d\sigma}{dT} \) describes the temperature coefficient of surface tension of SS316L. The recoil vapor pressure \( P_r \) is defined as [31]
\[ P_r = 0.54 P_0 \exp \left[ \frac{L_M (T - T_e)}{RT_v} \right] \frac{n | \nabla \alpha |}{n | \nabla \alpha |} \frac{2 \rho}{\rho_{\text{metal}} + \rho_{\text{gas}}} \]  

(12)

where \( P_0 \) is the ambient pressure, \( L_v \) is the latent heat of vaporization, \( T_v \) is the evaporation temperature, \( M \) is the molar mass, \( R \) is the universal gas constant.

For the conservation of energy, one can express as [21]

\[ \bar{p} C_p \left( \frac{\partial T}{\partial t} + \bar{u} \cdot \nabla T \right) = -\alpha \rho_{\text{metal}} L_m \left( \frac{\partial \gamma}{\partial t} + \bar{u} \cdot \nabla \gamma \right) + \nabla \cdot \left( \bar{k} \nabla T \right) + q_v + q_{\text{rad}} + q_{\text{laser}} \]  

(13)

where \( C_p \) is the specific heat capacity, \( L_m \) is the latent heat of melting, \( \bar{k} \) is the mixture thermal conductivity, \( q_v \) is the heat loss due to evaporation, \( q_{\text{rad}} \) is the heat loss due to radiation, \( q_{\text{laser}} \) is the heat input from the laser beam. The first term in the right hand side (RHS) describes the enthalpy change due to melting. The evaporation heat loss is defined as [31]

\[ q_v = -0.82 \frac{L_M}{\sqrt{2 \pi MRT}} P_0 \exp \left[ \frac{L_M (T - T_e)}{RT_v} \right] \frac{2 \rho C_p}{\rho_{\text{metal}} C_{\text{metal}} + \rho_{\text{gas}} C_{\text{gas}}} \]  

(14)

The term \( \frac{2 \rho C_p}{\rho_{\text{metal}} C_{\text{metal}} + \rho_{\text{gas}} C_{\text{gas}}} \) plays a similar role with the multiplier term mentioned above.

The radiation heat loss is given by [21]

\[ q_{\text{rad}} = -\sigma_s \varepsilon (T^4 - T_{\text{ref}}^4) \frac{2 \rho C_p}{\rho_{\text{metal}} C_{\text{metal}} + \rho_{\text{gas}} C_{\text{gas}}} \]  

(15)

where \( \sigma_s \), \( \varepsilon \), \( T_{\text{ref}} \) are the Stefan-Boltzmann constant, emissivity and ambient temperature, respectively.

The moving laser beam is described by a Gaussian distribution [32]

\[ q_{\text{laser}} = -\sigma_s \varepsilon (T^4 - T_{\text{ref}}^4) \frac{2 \rho C_p}{\rho_{\text{metal}} C_{\text{metal}} + \rho_{\text{gas}} C_{\text{gas}}} \]
\[ I = \frac{2 \xi P}{\pi r^2} \exp \left[ -2 \left( \frac{(x + v_0 t - x_0)^2 + (z - z_0)^2}{r^2} \right) \right] \]  

(16)

where \( I \) is the beam power density, \( P \) is the laser power, \( \xi \) is the absorption coefficient, \( r \) is the beam radius, \((x_0, z_0)\) describes the starting position of the laser beam, \( v_0 \) denotes the scanning velocity. Due to the concern of computational cost, our model ignores the Fresnel reflections of the laser beam [33, 34]. The incorporation of Fresnel absorption may further improve the accuracy of the simulation results. In the current study, the laser power was only absorbed by the top free surface of the workpiece. Similar to previous work by Korner et al. [17], when a bundle of laser ray touches a powder particle or the melt pool, the laser power is absorbed by the corresponding numerical grid. An index \( f_{\text{absorb}} \) ranging from 0 to 1 was calculated to track the top surface of the workpiece. Therefore, the heat input from the laser beam is approximated as

\[ q_{\text{laser}} = \frac{f_{\text{absorb}} I}{\Delta y} \]  

(17)

where \( \Delta y \) represents the size of the numerical grid. By solving the set of Eqns. (1), (5), (6) and (13), the evolution of melt flow during AM can be rationalised.

The 3D computation domain with size of 1000×400×200  \( \mu \text{m}^3 \) was employed to perform the simulation, as shown in Figure 1. The domain consisted of a 200-\( \mu \text{m} \) tall substrate, a 50-\( \mu \text{m} \) tall powder layer and a 150-\( \mu \text{m} \) tall gas region to track the free surface during laser scanning. The powder layer was initialized by importing the particle coordinates and sizes calculated from the DEM method. The analytical domain was divided into a regular Cartesian grid with a mesh size of 2.5×2.5×2.5  \( \mu \text{m}^3 \), yielding about 5 million cells in the simulation. The initial temperature was set to be 300 K to incorporate the ambient temperature. Boundary conditions
for all the surfaces were considered as continuative (zero normal derivative). SS316L was selected as the simulation material. The thermophysical properties of SS316L [35, 36] and the various constants applied in the simulation are summarized in Table 1. The heat source parameters are tabulated in Table 2. The CFD model was validated against the experimental results by Kamath et al. [25], as shown in Figure S1 and Table S1.

![Computational domain used to simulate the single-track formation](image)

Figure 1. Computational domain used to simulate the single-track formation: (a) three-dimensional configuration, and (b) the longitudinal cross section view. The translucent grey
box denotes the gas layer above the powder bed. The red arrows represent the scanning direction of the laser beam.

Table 1. Thermophysical properties of SS316L and coefficients applied in the simulation.

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density of solid metal (kg m(^{-3}))</td>
<td>(\rho_s)</td>
<td>8084-0.42097-3.894\times(10^{-5})(T^2)</td>
</tr>
<tr>
<td>Density of liquid metal (kg m(^{-3}))</td>
<td>(\rho_l)</td>
<td>7433-0.03937-1.8\times(10^{4})(T^2)</td>
</tr>
<tr>
<td>Specific heat of solid metal (m(^2) s(^{-2}) K(^{-1}))</td>
<td>(C_{ps})</td>
<td>462+0.134 (T)</td>
</tr>
<tr>
<td>Specific heat of liquid metal (m(^2) s(^{-2}) K(^{-1}))</td>
<td>(C_{pl})</td>
<td>775</td>
</tr>
<tr>
<td>Thermal conductivity of solid metal (kg m(^{-3}) s(^{-1}) K(^{-1}))</td>
<td>(k_s)</td>
<td>9.248+0.01571(T)</td>
</tr>
<tr>
<td>Thermal conductivity of liquid metal (kg m(^{-3}) s(^{-1}) K(^{-1}))</td>
<td>(k_l)</td>
<td>12.41+0.003279(T)</td>
</tr>
<tr>
<td>Solidus temperature (K)</td>
<td>(T_s)</td>
<td>1658</td>
</tr>
<tr>
<td>Liquidus temperature (K)</td>
<td>(T_l)</td>
<td>1723</td>
</tr>
<tr>
<td>Evaporation temperature (K)</td>
<td>(T_v)</td>
<td>3090</td>
</tr>
<tr>
<td>Latent heat of melting (m(^2) s(^{-2}))</td>
<td>(L_m)</td>
<td>2.7\times(10^5)</td>
</tr>
<tr>
<td>Latent heat of vaporization (m(^2) s(^{-2}))</td>
<td>(L_v)</td>
<td>7.45\times(10^6)</td>
</tr>
<tr>
<td>Viscosity of liquid metal (kg m(^{-1}) s(^{-1}))</td>
<td>(\mu_l)</td>
<td>10((2358.2/T-3.5958))</td>
</tr>
<tr>
<td>Surface tension (kg s(^{-2}))</td>
<td>(\sigma)</td>
<td>1.6</td>
</tr>
<tr>
<td>Temperature of surface tension (kg s(^{-2}) K(^{-1}))</td>
<td>(d\sigma/dT)</td>
<td>0.8\times(10^{-3})</td>
</tr>
<tr>
<td>Permeability coefficient (kg m(^{-3}) s(^{-1}))</td>
<td>(K_e)</td>
<td>1\times(10^6)</td>
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<tr>
<td>Molar mass (kg mol(^{-1}))</td>
<td>(M)</td>
<td>0.05593</td>
</tr>
<tr>
<td>Ambient pressure (kg m(^{-1}) s(^{-2}))</td>
<td>(P_0)</td>
<td>101000</td>
</tr>
<tr>
<td>Universal gas constant (kg m(^3) s(^{-2}) K(^{-1}) mol(^{-1}))</td>
<td>(R)</td>
<td>8.314</td>
</tr>
<tr>
<td>Stefan-Boltzmann constant (kg s(^{-3}) K(^{-4}))</td>
<td>(\sigma_s)</td>
<td>5.67\times(10^8)</td>
</tr>
<tr>
<td>Emissivity</td>
<td>(\varepsilon)</td>
<td>0.26</td>
</tr>
</tbody>
</table>

Table 2. Data used for the heat source in this simulation.

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam radius ((\mu)m)</td>
<td>(r)</td>
<td>27</td>
</tr>
<tr>
<td>Scanning speed (m/s)</td>
<td>(v_0)</td>
<td>0.75, 1.5, 3.0, 6.0</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>(\xi)</td>
<td>0.35</td>
</tr>
<tr>
<td>Total beam power (W)</td>
<td>(P)</td>
<td>50, 100, 200, 400</td>
</tr>
</tbody>
</table>

3. Results and discussion

3.1. Anatomy of a single track without defects
(a)

$t = 160 \mu s$

Cutting plane for (b)

$t = 320 \mu s$

Solid Melt pool

$t = 500 \mu s$

Partially melted particles Depression

$t = 634 \mu s$
Figure 2. Time snapshots showing the evolution of the melt track ($P=200$ W, $v=1.5$ m/s): (a) top view, and (b) longitude cross section view. The cross sections are sliced at the beam centre ($z = 100$ μm). The temperature distribution during SLM is represented by the colour scheme, which is also used in other figures. The liquid melt pool is confined within the black contour line ($T > 1723$ K). The laser denoted by the vertical thick line is turned off at 533 μs.

A laser power of 200 W and a scanning speed of 1.5 m/s were applied to carry out the first simulation. The starting point of the laser beam centre is located at $(x_0, z_0) = (100, 100)$ μm.
The entire heating duration was set as 533 μs, yielding a scanning length of 800 μm. Thereafter the heat source was removed for another 100 μs to cool down the system.

A continuous track is formed with such processing conditions, as illustrated in Figure 2. According to the figure, powder particles near the laser beam are heated up and fully melted. Similar to the coalescence of water droplets, the surface tension force causes the rapid fusion of melted particles [20]. Meanwhile, the substrate below the powder layer is also melted, as can be seen in the black contoured region in Figure 2(b). Driven by surface tension, the nearby melted particles are pulled towards the base plate, which is known as the “wetting” effect [37]. As a result, the molten materials tend to spread steadily across the substrate surface, leading to the good bonding between the melted portion and the substrate. A continuous track welded with the base plate is thus formed by the coalescence of melted particles and the wetting behaviour. Such phenomenon is nature’s manifestation of minimizing surface energy and surface area.

Additionally, a depression region can be clearly observed near the laser beam spot during SLM processing. With surface temperatures reaching the boiling point (red region), the recoil vapor pressure becomes predominant and exerts a downward force upon the top surface, pushing out the molten metal and creating a depression/concave zone. The depression momentum is indicated by the downward velocity vectors near the laser spot (Figure 3(b)). The liquid metal quickly flows back into the concave region when the heat source moves to next position, which is attributed to the rapid drop of recoil pressure induced by the decrease of local temperature. Under the effect of surface tension and hydrostatic pressure, the molten metal located on the upper part of the depression region starts to flow towards the centre of the concave cavity. The reversal motion of liquid metal is represented by the inward velocity vectors right after the laser beam (Figure 3(b)). With the formation and collapse of the depression site, the complex motion of molten materials causes melt pool instability near the laser beam spot, which is believed to
be the fundamental origins of structural defects and non-uniformity of the solidified tracks [6]. Such phenomenon observed in our simulation is closely related with the keyhole formation and collapse observed in laser welding [38, 39]. Despite the different geometrical features of SLM and laser welding, one should note that the physical mechanisms of them are considerably similar. Moreover, the concave region at the end of the track remains upon switching off the heat source, as demonstrated by the snapshots taken at 634 μs in Figure 2. The retention of keyhole cavity results from the fast cooling after the laser is switched off at 533 μs, leading to the rapid consolidation of molten metal at the end. This behaviour exhibits agreement with the inclination of keyhole front reported by Eriksson’s laser welding experimentation [40]. Similar features can be observed in SLM experiment [41, 42] and simulation [19].
Figure 3. (a) Longitudinal 2D slices of the track at different positions ($z = 110$ and $120 \, \mu m$), showing whether porosities are induced with 200 W power and 1.5 m/s scanning speed. (b) The enlarged melt pool at 500 $\mu s$. The arrows denote the velocity vectors of the molten materials. The liquid melt pool is confined within the black contour line ($T > 1723$ K).

As shown by the snapshots at 500 $\mu s$ in Figures 2(b) and 3(a), the longitudinal cross sections of the model were extracted to examine whether porosities are generated during the melting and solidification process. In Figures 2(b) and 3(a), the longitudinal cross sections were sliced.
at \( z = 100, 110, \) and \( 120 \ \mu m \), respectively. The slice at \( z = 100 \ \mu m \) corresponds to the centre of the laser beam, whereas the slice at \( z = 120 \ \mu m \) is close to the edge of the laser beam (beam radius is \( 27 \ \mu m \)). As observed in these three slices, the absence of porosity denotes the formation of a solidified track with few structural defects. Accordingly, the power of 200 W and scanning speed of 1.5 m/s are appropriate parameters to eliminate porosity development in the SS316L single track.

In this case, the minimization of structural defects can be ascribed by two aspects. Firstly, the input energy is sufficient to melt the base plate below the powder layer. The resultant wetting effect promotes the spreading of liquid metal on the baseplate surface, leading to the perfect bonding between the consolidated track and the substrate. The wetting behaviour is beneficial to avoid interlayer flaws. Secondly, the depression zone depth is found to be relatively small during the scanning process (see Figures 2(b) and 3(b)). For the shallow depression, the liquid metal in the rear part of the melt pool can quickly fill up the depression site during laser scanning (except for the end of the track), thereby avoiding the possibility of entrapped gas within the consolidated sample. The wetting behaviour and shallow depression together contributes to the formation of a porosity-free track. In addition, the melt pool depths are found to vary with the slice locations (see Figure 3(b)). Such difference can be directly attributed to the Gaussian distributed energy intensity. It can be easily noted that the energy intensity is highest at the beam centre (\( z = 100 \ \mu m \)). Therefore, the melt pool depth should gradually decrease from the beam centre to the edge.

3.2. Porosity induced by keyhole formation and collapse
Figure 4. Simulation results of the track produced at $P=400$ W, $v=1.5$ m/s: (a) top view at 634 μs, and (b) cross sections at 500 μs. The liquid melt pool is confined within the black contour line ($T > 1723$ K). The laser creates a deep and narrow keyhole during SLM. Near-spherical cavities can be observed near the melt pool bottom.
With the same powder layer configuration in Section 3.1, the laser power was increased to 400 W and the scanning velocity is still 1.5 m/s. The top view at 634 μs and cross section snapshots at 500 μs are depicted in Figures 4 (a) to (d). Compared with the power of 200 W, it is clearly observed that the solidified track processed with 400 W is highly distorted and irregular. A similar phenomenon was observed in Trapp’s work [41] on the SLM of aluminium powders. The distortion of the solidified track probably results from the melt pool instability, as a deep keyhole quickly forms and collapses near the beam spot. It also becomes evident that the excessive input energy introduces near-spherical porosities underneath the solidified track, sharing the similar traits with experimental observations [13]. Figure S2 shows the 3D distribution of near-spherical porosities within the solidified sample.
Figure 5. The formation process of keyhole porosity during high power SLM: (a) $t = 422 \ \mu$s, (b) $t = 426 \ \mu$s, (c) $t = 428 \ \mu$s and (d) $t = 460 \ \mu$s. The black arrows denote the fluid velocities in the melt pool. The liquid melt pool is confined within the black contour line ($T > 1723 \ \text{K}$).

The formation mechanisms of near-spherical porosities in high power SLM are similar to the keyhole mode laser welding process [43-45]. During high power SLM process, the flow patterns within the melt pool are strongly affected by the competition between the surface tension and the recoil pressure and other factors. The evaporation-induced recoil pressure can greatly depress the melt pool and maintains the keyhole open. On the other hand, the surface tension tends to minimize the surface area and prevent the keyhole formation. Due to the competitive effects of various dynamic forces in the melt pool, the flow behaviour in the melt pool is highly unstable and can induce the bubble formation during the laser scanning process. The entrapment of gas bubbles can cause the development of near-spherical porosities during SLM.

The complex and unsteady flow patterns in the melt pool are shown in Figure 5, where the temperature distribution and fluid velocity are also given. As the laser beam is a moving heat source, a thin layer of liquid metal can be observed in the front keyhole wall. Driven by the recoil vapor pressure, the molten liquid in the front keyhole wall is observed to flow downwards along the gas/metal interface. On the other hand, the flow behaviour in the rear part of the melt pool is highly unstable and complex, as illustrated in Figure 5(a). It can be noticed that the liquid metal flows downwards near the top surface behind the keyhole, which is mainly caused by the recoil pressure and surface tension. As the molten liquids reach the bottom at the solid/liquid boundary, the molten materials are directed rearward along the fusion line (the black contour line), leading to the formation of a clockwise vortex in the rear part of the melt pool. In addition, the fluid velocity around the keyhole is more drastic than the other parts of the melt pool, indicating the intense and unsteady flow patterns near the keyhole. The flow
patterns of high power SLM are consistent with the keyhole model laser welding process [44, 45], and the unstable flow behaviour in the rear part of the melt pool could give rise to the bubble formation during the laser scanning process.

Figures 5(a) to (d) illustrate the formation process of an entrapped bubble during high power SLM process, demonstrating the physical mechanisms of near-spherical porosities observed in additively manufactured samples. At \( t = 422 \mu s \), it can be seen that the molten liquids behind the upper rear keyhole wall flow towards the front keyhole wall. Such phenomenon is primarily driven by the strong clockwise vortex in the melt pool, as discussed by previous simulations of keyhole laser welding [43, 45]. As a result \((t = 426 \mu s)\), a hump (or bulge) caused by the back flow of melt is formed at the rear wall of the keyhole. The hump may collapse due to the severe oscillation and instability of the keyhole, forming enclosed gas bubble at the keyhole bottom \((t = 428 \mu s)\). If the entrapped gas bubble fails to escape from the melt pool, near-spherical porosity would be induced after solidification \((t = 460 \mu s)\). Based on the numerical analysis, the development of keyhole porosities is closely related to the unsteady flow behaviours near the rear part of the keyhole, which is also characterized by the strong clockwise vortex.

Nevertheless, it should be emphasized that a gas bubble in the melt pool may not result in the formation of porosity after solidification. It is possible for a gas bubble to merge back with the keyhole during laser scanning. Additionally, gas bubbles can escape from the top surface of the melt pool, which is associated with the migration of gas bubbles. A possible reason for the migration of gas bubbles is the clockwise vortex of liquid metal in the melt pool. Driven by the surrounding flow patterns of molten liquids, gas bubbles tend to move backwards and upwards during the laser scanning process. On the other hand, buoyance force can cause the upwards migration of gas bubbles, as the density of gas is significantly smaller than the molten liquids. Due to the upward migrations, some gas bubbles can float out from the top surface.
Accordingly, only those entrapped gas bubbles lead to the development of near-spherical porosities in the solidified metal.

The simulation results with high energy input clearly reveal the formation mechanisms of near-spherical porosities found in SLM specimens. Rather than the spherical pits [12] or open porosities [3] on the top surface, it is concluded that collapse of a deep keyhole causes gas entrapment during SLM fabrication, thereby creating near-spherical defects underneath the solidified track.

### 3.3. Porosity induced by lack of fusion

To better understand the formation mechanisms of irregular shaped defects, simulations were performed with laser power of 100 W and 50 W, respectively. The scanning speed remained 1.5 m/s.

Given a heat input of 100 W, the top view at 634 μs and cross sections at 500 μs are shown in Figure 6. The depression region almost vanishes due to the lower laser power. The top view at 634 μs suggests the formation of a continuous track with rough surface. At different positions (z = 100, 110 and 120 μm), the comparison of defect distribution and morphology is monitored by the longitudinal cross sections in Figures 6(b) to (d). At the laser beam centre (z = 100 μm), the energy intensity is marginally strong enough to melt the substrate below (see the black contour line in Figure 6(b)). The wetting behaviour thus takes place between the nearby melted particles and the substrate, building a continuous track after solidification. The wetting effect also alleviates the formation of interlayer defects, and hence few porosities are present at the beam centre. However near the beam boundary (z = 120 μm), the energy intensity is inadequate to melt the base plate below, and the melted particles tend to merge together rather than spread on the substrate. The absence of wetting behaviour therefore introduces interlayer flaws after the SLM process, as clearly illustrated in Figure 6(d). The presence of lateral porosities agrees
with experimental observations [11], and these defects are particularly detrimental to the mechanical performance of built samples. Despite the formation of a continuous track, the track with 100 W power displays the presence of interlayer flaws near the beam edges, which is attributed to the Gaussian distributed heat source. A possible approach to diminish these defects is to appropriately adjust the hatch spacing, which was suggested by Thijs et al.[46].
Figure 6. Simulation results of the track produced at $P=100$ W, $v=1.5$ m/s: (a) top view at 634 $\mu$s, and (b) cross sections at 500 $\mu$s. The liquid melt pool is confined within the black contour line ($T > 1723$ K). The track has a rough surface. Interlayer porosities due to the lack of wetting behaviour can be seen near the beam edge.
Figure 7. Simulation results of the track produced at $P=50$ W, $v=1.5$ m/s: (a) top view at 634 $\mu$s, and (b) cross sections at 500 $\mu$s. The liquid melt pool is confined within the black contour line ($T > 1723$ K). The track can be characterized by discontinuous balls.
Previous experiments reported balling effects in SLM with insufficient laser power or high scanning speed [47]. Similarly, the current investigation suggests the formation of a discontinuous track with extra low power (50 W), as given by Figures 7. In this study, the balling effect is found to result from the lack of fusion and wetting behaviour. Even at the beam centre with highest energy intensity (see the black contour line in Figure 7(b)), the below substrate remains unmelted due to the low laser power. Without the wetting behaviour, the melted particles thus prefer to coalesce with neighbouring powders as small droplets, and then rapidly consolidate into individual balls. It is commonly believed that the balling effect in SLM comes from the so-called Plateau-Rayleigh instability, which demonstrates that the surface tension breaks a long melt track into isolated droplets to minimize the surface area [20]. The presence of Plateau-Rayleigh instability may be suppressed by the wetting behaviour [15]. Our simulation results prove that an extra low power completely prevents the wetting behaviour between the substrate and those melted particles, and the droplets formed by particle coalescences account for the isolated balls found in SLM specimens. Therefore, the single track discontinuity and existence of irregularly shape porosities are possibly attributed to the absence of wetting behaviour induced by lack of melting.

3.4. Effects of scanning speeds

The above sections provide a comprehensive discussion on the influences of laser power. To further understand how scanning speed affects the quality of as-built samples, additional laser speed of 0.75, 3.0 and 6.0 m/s were selected as contrastive parameters to perform simulations. The power was kept at 200 W. The heating duration was respectively set as 1066, 266 and 133 μs, yielding the same scanning length of 800 μm. As illustrated by Figures S3 to S5, it is noted that the effect of decreasing scanning speed is similar with that of increasing laser power. Such phenomenon tallies with experimental observations [9, 47], and the physical mechanisms are clarified in previous sections. The sample fabricated with scanning speed of 0.75 m/s retains
near-spherical porosities (see Figure S3), which could be ascribed by the keyhole collapse. High scanning speeds worsen the wettability between the powder layer and the substrate, giving rise to the interlayer flaws with irregular patterns.

3.5. Multilayer simulation

As aforementioned, the analyses of single track elucidate the formation mechanisms of near-spherical and irregularly shaped defects with varying laser parameters. This section investigates the SLM processing of the second layer of metal particles, revealing how porosities accumulate through the layer-by-layer manner.

After the solidification of the first melt layer (at 634 µs), the surface geometries of the solidified models were extracted as STL files. A second layer of metal powders were then deposited on the solidified beds through DEM approach. Similar to the procedure described in Section 2.1, the recoating blade was applied to pass over the second layer of metal powders, ensuring a distance of 100 µm between the top surface of the powder bed and that of the initial substrate. Thereafter we employed the CFD model to simulate the SLM processing of the second layer. One can repeat such process to monitor the fusion between consecutive layers. The initial configurations of the second layer of particles together with the solidified beds are illustrated in Figure 8.
Figure 8. 2D slices of the second powder layer deposited on the solidified tracks. In (a) to (d), the prior consolidated beds are fabricated by the power of 400, 200, 100 and 50 W, respectively. The horizontal black lines demonstrate the top surface of the second powder layer. The red contour lines represent the configurations of previously solidified layers.
Figure 9. Simulation results of the second layer track produced at $P=200$ W, $v=1.5$ m/s: (a) top view at 634 $\mu$s, and (b) cross sections at 500 $\mu$s. The red contour lines represent the top surface of the first layer. The liquid melt pool is confined within the black contour line ($T > 1723$ K). Interlayer defects can be observed near the edge of the laser beam.
With a power of 200 W and a scanning speed of 1.5 m/s, simulation of laser scanning was performed on the second layer of powder bed. Figure 9 shows the top surface and cross sections of the model. The snapshot at 634 μs denotes the geometry of the consolidated track, while the heat source is still applied on the model at 500 μs. In Figures 9(b) to (d), the red contour lines indicate the initial geometry of the previously solidified bed. At the beam centre (Figure 9(b)), the energy intensity is strong enough to remelt the top surface of the previous layer, which is evidenced by the melt pool denoted by the black contour line. Driven by the surface tension, the melted particles are fused together and bonded with previous layer, suppressing interfacial flaws between adjacent layers. Near the beam edges (Figure 9(d)), the previous layer is incompletely remelted, leading to the development of interlayer porosities. Comparatively, these defects are not observed during the laser processing of the first layer (Figure 4(d)).

Figure 10. 2D slice of the first layer track produced at $P=200 \text{ W}$, $v=1.5 \text{ m/s}$. The black circles represent the first powder layer before SLM. The horizontal black line represents the top surface of the first powder layer. The red contour line denotes the configuration of solidified track after laser processing. It is noted that the track height is smaller than the powder layer thickness, indicating that the thickness of second powder layer is greater than 50 μm.

Based on the simulation results, the porosities in Figure 9(d) is primarily due to the increased thickness of the second powder layer. As mentioned in Section 2, the thickness of the first powder layer is 50 μm. Due to the coalescence of melted particles, the voids originally existed between metal powders are filled up by the molten materials. The height of the solidified track
resultantly becomes less than 50 μm, as illustrated in Figure 10. As we deposit another layer of powders upon the solidified bed, the thickness of second powder layer would be greater than 50 μm in order to achieve a total 100 μm thickness. Due to the increased layer thickness, the energy intensity near the beam edge (Figure 9(d)) is inadequate to fully remelt the pre-existing layer, leaving interfacial porosities during laser scanning. Although the recoating blade position follows a stepwise increment of 50 μm, the powder layer thickness is found to be different. In our simulations, the first powder layer thickness is 50 μm, while the actual thickness of subsequent layers is greater than 50 μm. Such characteristics should also be emphasized in realistic experiments, as the layer thickness of SLM machines denotes the stepwise descending of the platform/substrate.

Another factor affecting the distribution of interlayer porosities is the surface roughness of prior layer. The first powder layer thickness can be considered as a constant, since the top surface of the substrate is flat and smooth. Driven by the recoil pressure, surface tension and thermocapillary convection, the melt pool is forced to oscillate during SLM, resulting in a consolidated layer with rough surface (see the red contours in Figures 8 and 9). When we deposit another layer of powders upon the rough surface, the local powder thickness would fluctuate over the consolidated bed. A clear example can be seen in Figure 8(d). This disturbance of local powder thickness could be associated with the distribution of interlayer flaws. A locally thicker powder layer is likely to suppress the wetting behaviour and induce structural defects, since the energy intensity may be locally insufficient to remelt the pre-existing layer. Moreover, the surface roughness may deteriorate the melt pool instability of subsequent layers, thereby forming a consolidated bed with rougher surface [15]. Such viscous cycle may be responsible for the large flaws stretching over several layers.
Figure 11. Simulation results of the second layer track produced at $P=400$ W, $v=1.5$ m/s: (a) top view at 634 $\mu$s, and (b) cross sections at 500 $\mu$s. The liquid melt pool is confined within the black contour line ($T > 1723$ K). The red circles denote the locations of first layer porosities. New porosities arising from the collapse of second layer keyhole can be observed within the model.
With a higher power of 400 W, the processing results of the second powder layer are shown in Figure 11. Similar to the first layer, a deep keyhole penetrating the previous layer is formed during laser scanning. The resulting wetting behaviour eliminates the formation of interlayer porosities. On the other hand, new porosities are formed by the collapse of the deep keyhole. With excessive laser power (or low scanning speed) to process multiple layers, many keyhole porosities with random distribution and near-spherical patterns would be generated and accumulated within a sample. This phenomenon is evidenced by experimental observations [12]. In addition, it is noted that some trapped defects could be released during the prototyping of the next powder layer. The red circles in Figures 11(b) to (d) denote the positions of keyhole porosities formed after the processing of first layer. A portion of first layer porosities disappear (see the enclosed dashed boxes) during the second layer SLM, while the majority of them retain the locations and geometries within the model. For the first layer, the entrapped porosities are mostly present near the melt pool bottom (see Figures 4 and S2). Therefore, the moving keyhole of next layer (Figures 11(b) and (c)) is not deep enough to approach these porosities, resulting in the accumulation of seeded porosities. By contrast, those shallow porosities would be released (or reopen) by the keyhole penetration of next layer.
Figure 12. Simulation results of the second layer track produced at $P=100$ W, $v=1.5$ m/s: (a) top view at 634 μs, and (b) cross sections at 500 μs. The liquid melt pool is confined within the black contour line ($T > 1723$ K).
Processing results of second powder layer with power of 100 and 50 W are shown in Figures 12 and S6, respectively. As seen in Figure 12(b), interlayer porosities with irregular geometries are developed between the second powder layer and the solidified bed, which is not observed for the first layer (Figure 6(b)). These interfacial porosities are attributed to the increased power layer thickness and the surface roughness. With increased powder layer thickness, the prior bed undergoes partial re-melting during SLM, weakening the wettability between adjacent layers. In addition, the surface roughness of prior layer is liable for the fluctuations of local power layer thickness. For instance, it is noted that the enclosed region in Figure 4(c) corresponds to a concave area of the solidified bed, indicating a locally thicker powder layer near this site. A corresponding large porosity with encapsulated particles (Figure 12(c)) is found after the processing of second powder layer, since the power is not strong enough to penetrate the local powder layer. Defects with the same characteristic can be observed in literature [9]. Such phenomenon indicates that the surface faults (or roughness) of previous layer is important for the development of structural defects. Aboulkhair et al. [9] proposed that the porosity enclosing powders is related to keyhole, yet the present simulation study suggested a different mechanism.

The interactions between successive layers are discussed in this section. With excessive power, near-spherical porosities would be accumulated through the layer-by-layer manufacturing. The thickness of second powder layer is greater than 50 μm, influencing the wetting effect during SLM. The surface roughness of previously solidified layer also plays a role in determining the distribution of porosities, as the local powder thickness of next layer is forced to fluctuate by the rough surface.

4. Conclusion
With the high-fidelity powder scale model, this study clarifies the formation mechanisms of near-spherical and irregularly shaped defects during SLM. Through the single track simulations, the conclusions can be summarized as follows:

(1) Driven by surface tension, the melt track is formed by the fusion of melted powders and the wetting behaviour between melted powders and the substrate.

(2) Near-spherical porosities are entrapped gas bubbles arising from the collapse of a deep keyhole. This kind of structural defects are typically observed in the samples fabricated with high laser power or low scanning speed.

(3) Development of irregularly shaped porosities are fundamentally determined by the wetting behaviour. The wetting behaviour would be suppressed when the energy intensity is only strong enough to melt the powder layer rather than the substrate, giving rise to the formation of interlayer defects. The surface roughness of previously solidified layer is a key factor affecting the local thickness of next powder layer, which is related with the wettability and porosity development. Irregular-shaped porosities are generally formed with low laser power or high scanning speed.

(4) With insufficient melting, balling effect is primarily due to the absence of wetting effect.

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Conflict of interest

The authors declare that there is no conflict of interest.

References


