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

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C. Tang^a, J.L. Tan^{a,b}, C.H. Wong^{a,*}

a Singapore Centre for 3D Printing, School of Mechanical and Aerospace Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore ^b SLM Solutions Singapore Pte. Ltd., 25 International Business Park, #02-15/17 German Centre, Singapore 609916

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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.

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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 SLMprocessed materials, including residual stress [\[1\],](#page--1-0) crack [\[2\],](#page--1-0) microstructure [\[3,4\],](#page--1-0) mechanical properties [\[5\]](#page--1-0) and porosity [\[6,7\].](#page--1-0) 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 [\[8\].](#page--1-0) 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. [\[9\]](#page--1-0) 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. [\[10\]](#page--1-0) and Kaspeovich et al. [\[11\]](#page--1-0) 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. [\[12\]](#page--1-0) 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. [\[3\]](#page--1-0) observed open

[⇑] Corresponding author. E-mail address: chwong@ntu.edu.sg (C.H. Wong).

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. [\[13\]](#page--1-0) 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 at al. [\[15\]](#page--1-0) 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 [\[16\].](#page--1-0) Korner et al. [\[17\]](#page--1-0) 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. [\[18\]](#page--1-0) 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. [\[19,20\]](#page--1-0) 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. [\[6\]](#page--1-0) 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. [\[21\]](#page--1-0) noticed that the increment of layer thickness leads to the irregularity of scanned tracks. Lee et al. [\[22\]](#page--1-0) 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. [\[23\]](#page--1-0) 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 insitu 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) [\[24\]](#page--1-0) was adopted to model the random packing of SS316L particles laid on the solid substrate. Following the size distribution in Ref. [\[25\],](#page--1-0) the metal powders in this work are approximated as solid spheres with a mean diameter of $27 \mu m$ and a half maximum width of 10 um.

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 μ m high layer of metal particles, which is similar to the procedures reported in Ref. [\[26\]](#page--1-0). 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) [\[27\],](#page--1-0) 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 [\[28\]](#page--1-0) 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:

$$
\frac{\partial(\overline{\rho}\alpha_1)}{\partial t} + \nabla \cdot (\overline{\rho}\overrightarrow{u}\alpha_1) = 0 \tag{1}
$$

where \vec{u} is the flow velocity, t is time, \vec{p} is the volume-averaged density, α_1 is the volume fraction of metallic phase ($0 \le \alpha_1 \le 1$). α_1 = 1 indicates a cell completely occupied by the metallic phase, and α_1 = 0 corresponds to a gaseous cell where no metal is present. Additionally, any material property of mixture ϕ was computed

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