Computational modeling of selective laser melting process

Le, Kim Quy

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SINGAPORE

**COMPUTATIONAL MODELING OF SELECTIVE
LASER MELTING PROCESS**

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SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING

2020

COMPUTATIONAL MODELING OF SELECTIVE LASER MELTING PROCESS

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School of Mechanical and Aerospace Engineering

A thesis submitted to the Nanyang Technological University Singapore in the fulfillment of the
requirements for the degree of Doctor of Philosophy

2020

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research, is free of plagiarised materials, and has not been submitted for a higher degree to any other University or Institution.

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Supervisor Declaration Statement

I have reviewed the content and presentation style of this thesis and declare it is free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

1. August 2019
Date

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A/P DU HEJUN

Authorship Attribution Statement

This thesis contains material from two papers published in the following peer-reviewed journals and one paper in preparation in which I am listed as an author.

Chapter 4 is published as K. Q. Le, C. Tang, C. H. Wong, “A study on the influence of scanning strategies on the melt track and melt pool in selective laser melting process of stainless steel powder,” *JOM*, vol. 70, p. 2082-2087, 2018. DOI: 10.1007/s11837-018-2998-6.

The contributions of the co-authors are as follows:

- A/P Wong provided the project direction.
- The author performed the simulations with different scanning strategies using DEM model which was written by me and CFD model which was written by Dr. Tang.
- The CFD model was validated by the author, using her own experimental results.
- The author collected the simulation data and carried out the analyses together with A/P Wong.
- All the figures and plots, unless otherwise stated and referenced, were from the author’s simulated and experimental data.
- The author prepared the manuscript drafts. The manuscript was revised by Dr Tang and A/P Wong.
- A/P Wong submitted the paper to the journals.
- The author gave responses to the reviewers’ comments. The reply was revised by Dr. Tang Chao and A/P Wong.

Chapter 5 is published as K. Q. Le, C. Tang, C. H. Wong, “On the study of keyhole-mode melting in selective laser melting process,” *International Journal of Thermal Sciences*, vol. 145, p. 105992, 2019. DOI: 10.1016/j.ijthermalsci.2019.105992

The contributions of the co-authors are as follows:

- Dr. Tang suggested the idea in simulating the keyhole-mode.

- The author employed the CFD model which was written by Dr. Tang to run different keyhole-mode melt tracks. In addition, the simulated results were compared with her own experiments and the experiments of other groups.
- The author investigated the dynamics of the melt pool and found the existence of different fluid flows at different keyhole-modes and performed the analyses with A/P Wong.
- The author examined the pores in the simulation and in the experimental melt pool.
- All the figures and optical microscope images, unless otherwise stated and referenced, were from the author's simulated and experimental data.
- The author prepared the manuscript drafts. The manuscript was revised by Dr Tang and A/P. Wong.
- A/P Wong submitted the paper to the journals.
- The author gave responses to the reviewers' comments. The reply was revised by Dr. Tang Chao and A/P Wong.

Chapter 6 is in preparation for journal submission as K. Q. Le, K. H. G. Chua, C. Tang, and C. H. Wong, "Discontinuity in overhang melt- track in selective laser melting".

The contributions of the co-authors are as follows:

- The author suggested the idea in simulating the overhang after discussion with A/P Wong.
- The author modelled the powder bed with different overhanging features.
- The author employed the CFD model which was written by Dr. Tang to run different overhanging melt tracks, and collected the simulation data.
- Mr. Chua and the author printed the samples and performed polishing and etching.
- Digital optical images were taken by Mr. Chua.
- All the figures were prepared by the author, while the analyses were performed by the author and A/P Wong.
- The author prepared the manuscript drafts. The manuscript was revised by Mr. Chua, Dr Tang and Prof. Wong.

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ABSTRACT

Selective laser melting (SLM) is a metal-based additive manufacturing (AM) process which can produce printed parts with high density and good mechanical properties. However, the properties of the printed part depend on several processing parameters including laser power, scanning speed, layer thickness, powder distribution, and hatch spacing. Moreover, SLM is a multi-physics process, including heat transfer, fluid flows, multi-phase interactions, phase-change process, laser-material interaction, and chemical reactions. In order to model and simulate the SLM process correctly, several methodologies have to be adopted. Discrete element method (DEM), which is a finite-difference method widely used for simulating granular systems, has been applied to describe the Newtonian interactions of the particles (or powders) in SLM, while computational fluid dynamics (CFD) has been adopted to model the thermodynamics of the melting process.

In this work, open-source software packages including LIGGGHTS[®] and OpenFOAM[®] were chosen to simulate the SLM process. LIGGGHTS[®] is a DEM solver and OpenFOAM[®] is a CFD solver. The heat transfer, fluid flows, laser-material interaction, phase-change, and multi-phase interactions were all performed in OpenFOAM[®].

A model has been developed to simulate the deposition of powder, the melting process, and the solidification of the melt track. Moreover, multi-physics in SLM process have been imitated, including heat transfer, fluid dynamics, phase-change, multi-phase interaction, and the interaction of the laser beam with the powder bed. Different forces, such as surface tension, recoil pressure, and Marangoni force, have been presented. Two models for the laser beam source has been developed – as a simplified heat source and one that mimics the multiple reflections by

employing a ray-tracing model. Both models have been validated by comparing the melt pool depths and widths of the simulation to experiments.

The laser beam, when simulated as a simplified heat source, was applied on the top surface of the powder bed. The simplified heat source model was employed to examine the levelness of the melt tracks produced with different scanning patterns. The study found that the sequential scanning pattern leads to a non-flat printed surface, while the boustrophedon pattern produces a flat printed surface.

Multiple reflections of the laser beam have been developed by employing the ray-tracing model to simulate the keyhole-mode melting phenomenon. The melt pool can be in conduction-, transient-, or keyhole-mode. In the study, the melt pool is considered to be in conduction-mode when the ratio of the melt pool depth to the melt pool width is less than 0.5 and keyhole-mode when the ratio is above 1.0. The region between the conduction-mode and the keyhole-mode is known as the transient-mode. Although the simplified heat source model was able to simulate the conduction-mode melting with results close to the experiments, it is inadequate for keyhole-mode melting which requires the representation of multiple reflections of the laser beam to be included. As such, the ray-tracing model was developed to simulate the keyhole-mode and the melt pool dynamics of the keyhole-mode melt track. Furthermore, the model offers a channel to predict the keyhole-induced porosities in the solidified melt track.

Hence in this study, two types of keyhole-mode melting were investigated, namely medium-deep keyhole and well-deep keyhole. When the ratio between melt pool depth and melt pool width

was greater than a reference value of 1.5, it can be considered as the well-deep keyhole. The study found that the melt pool dynamics of the well-deep keyhole is unsteady as compared to the medium-deep keyhole. Different modes of fluid flow, such as downward flow, bottom backward flow, clockwise flow and top forward flow are noticed in the well-deep keyhole melt pool. On the other hand, the melt pool dynamics of the medium-deep keyhole is more stable with two main flows: the downward flow and backward flow. In addition, the ray-tracing model was also employed to investigate the melt track morphology of the overhanging structure. The study found that the overhanging melt track often experiences discontinuity due to wetting effect, low surface tension gradient. In addition, short lifetime of the melt pool also leads to the discontinuity, where the lifetime of a melt pool was estimated from the time when the material was melted until it was fully solidified. However, by applying high laser power while maintaining low energy density alleviates the discontinuities and at the same time achieves high geometrical accuracy of the overhanging printed part.

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CHAPTER 1: INTRODUCTION

1.1. Background of additive manufacturing

Additive manufacturing (AM), which is also known as three-dimensional (3D) printing, is slated to be a major component in the fourth industrial revolution. The history of AM began in 1987 when the first commercial AM system (StereoLithography apparatus 1) was introduced to the world [1]. By 1991, three AM technologies including fused deposition model (FDM), solid ground curing (SGC), and laminated object manufacturing (LOM) were commercialized [1, 2]. In 1992, selective laser sintering (SLS) became available [1]. Since then, many new AM systems were introduced such as the multi-colour 3D printer, direct metal deposition (DMD) technology, digital light processing (DLP), and powder bed fusion (PBF) process.

AM is not a single process. Instead, it is a collection of fabrication methodologies. The processes differ depending on the material and technology used. In 2010, ASTM F42 subcommittee classify the range of AM processes into seven categories including vat photopolymerization, material jetting, binder jetting, material extrusion, PBF, sheet lamination, and DED. Table 1.1 summarises the different AM processes [3].

In the vat photopolymerization process, which has been used in biomedical and prototyping applications, an ultraviolet light source is employed to cure the resin and the part is printed layer upon layer to form a high quality and high resolution 3D object [3]. However, this process is slow and is generally limited to materials such as a dispersion of ceramic-polymer composites or polymer-derived ceramifiable monomers [4, 5] On the contrary, in the material jetting process,

concentrated droplets of material, such as ceramic, concrete or soil in the form of liquid ink or paste, are deposited layer upon layer to print large scale parts quickly albeit with poor resolution due to poor bonding between the layers [6]. This method has been adopted in biomedical and building and construction applications. Like the material jetting process, the material extrusion process is available only to a limited number of materials – thermoplastics and concrete. In this process, material is continuously pushed out of the nozzle layer after layer to form a printed part simply and quickly [6, 7]. A very commonly known material extrusion process is the FDM.

In binder jetting process, liquid bonding ink is deposited at the selective region to join solid powder material. Although the process is suitable for different materials such as metals, alloys, and ceramics [8], and does not require any support structure [9], the printed part usually exhibits high porosity [6]. Another AM technology in which a wide range of materials has been adopted is the sheet lamination process. In this process, materials sheets made of paper, metal, ceramics or polymer are bonded together. Then, a knife or laser was employed to cut in each layer to form a desired 3D part while reducing tooling and manufacturing time [8]. Unfortunately, the process is limited to printing simple parts with low geometrical accuracy [6].

Another popular AM technology is the PBF process in which thermal energy is employed to fuse selected regions of powder bed [8]. Although the PBF process is slow and costly, it is able to print high resolution parts with high density and whose mechanical properties are comparable to those produced by traditional methods. The PBF process has been widely used and some of the materials used include metals, alloys and ceramics [6]. Common processes of PBF are selective laser sintering (SLS), selective laser melting (SLM) and electron beam melting (EBM).

In the DED process, the material can be in the form of powder or wire [8]. The nozzle of thermal energy can move in multiple directions to melt the material which was deposited in different angles [10]. The process is widely used in the repair industry because deposition can be performed on existing parts. Furthermore, the process produces parts with excellent mechanical properties. However, parts produced by DED usually possess low geometrical accuracy and surface quality. This limits the process to printing only simple shapes.

Table 1.1: The classification of AM processes [3]

AM process	Description	AM techniques	Materials
Vat photopolymerization	A light source is employed to cure liquid photopolymer	SLA	Radiation-curable resins
Material jetting	The liquid material is dropped layer by layer to form 3D part.	Inkjet printing	Polymers, metals, ceramics
Binder jetting	Liquid bonding ink is deposited at the selective region to join solid powder material	3D printing (3DP)	Polymers, metals, ceramics
Material extrusion	Material is extruded through a nozzle	FDM	Polymer, ceramics

Powder bed fusion	High thermal energy is employed to selectively melt the powder bed	SLS, SLM, EBM	Polymers, metal, ceramics
Sheet lamination	Materials sheets are bonded together, then a knife or a laser beam is employed to cut in each layer to form a desired 3D part	LOM	Paper, metals, ceramics, polymers
Directed energy deposition	The nozzle of thermal energy can move in multiple directions to melt the material which was deposited in different angles	Laser engineered net shaping (LENS), DMD	Metals

Despite the differences in the AM processes, they generally follow the same workflow as shown in Figure 1.1. A 3D model is first created using computer aided design (CAD) software before digitally slicing the model into many thin layers. In current AM practice, the common technique for slicing is to produce contour data from STereoLithography (STL) files. Another technique is direct slicing from original CAD models which may alleviate any errors and the need for the repairing process of STL files [11]. After that, the sliced contours are exported to the AM system in which the input parameters such as materials, energy source, and layer thickness are set. The

fabrication then begins and when the part is completely printed, it will be removed from the substrate for post-processing such as surface treatment before putting the part in service.

Figure 1.1: General AM process steps [12].

Additionally, AM has been adopted in a myriad of applications such as aerospace, automotive, biomedical, digital art, and architecture design [9]. In 2017, aerospace comprised 18.2% in the AM market [13]. Different AM technologies have been employed in the aerospace industry. For instance, while DED was employed to print the helicopter engine combustion chamber, the SLS process was used to print the satellite antenna bracket [13]. Additionally, FDM has been adopted to print door handles in Boeing 777-300ER airplanes, and other technologies such as SLA and binder jetting have also been used in the aerospace industry [13]. Moreover, with the advancement in biomaterials science and biomedicines, the employment of AM in the biomedical industry has increased. Additively manufactured biomedical implants, for example, have been developed and certified for use. For instance, Adler Ortho Group launched the CE-certified Fixa Ti-Por acetabular cup produced by the EBD technique with more than 2000 of these cups have been implanted in 2007 [9]. Besides that, Ti6Al4V acetabular cups implants with purposefully designed porosity and dental prosthesis have been successfully printed [9]. Furthermore, AM also has begun to make an impact on the building and construction industry. For example, the Dubai Future Foundation office was printed in Shanghai and shipped to Dubai for assembly [14].

1.2 Motivations

1.2.1. The SLM process in metal-based additive manufacturing

SLM is one of the PBF technologies widely adopted by the industries [15]. It is capable of building parts at very high density, generally above 99% in comparison to conventional manufacturing, since the particles are fully melted during the fabrication process [16]. Moreover, printing parameters have been optimised to achieve a density of 99.7% with SLM Waspaloy[®] specimens powder [17]. Furthermore, SLM is reported to produce parts with high quality mechanical properties under suitable printing process parameters [16]. For instance, Wang *et al.* found that SLM is able to produce IN718 printed part which has tensile strengths and ductility comparable to those of the wrought IN718 [18]. Additionally, Sun *et al.* showed that it is possible to increase the building rate of SLM process by 72% by employing higher laser powder and faster scanning speed [19]. Moreover, in the study by Vrancken *et al.*, it was shown that heat treatment of Ti-6Al-4V can improve the mechanical properties of SLM parts to as close as those produced via conventional processes [20].

Furthermore, different materials including metals, alloys, ceramics and composites can be used in the SLM process [21]. Steels, titanium, titanium-based alloys, nickel-based alloys, aluminium-based alloys, magnesium, cobalt-chrome, tungsten are common metals and alloys that have been used and studied [22-28]. As liquid Titanium is sensitive to oxygen, nitrogen, hydron and carbon, it is challenging to fabricate Titanium part by employing conventional manufacturing [21, 23]. However, all these issues can be solved by employing the SLM process since the chamber is working in an inert gas environment filled with argon or nitrogen. Moreover, selectively laser melting of parts made of ceramics such as Li₂O-Al₂O₃-SiO₂ glass, silica (SiO₂), and alumina-

zirconium have been investigated [29-31]. Furthermore, composite materials are also printable by employing the SLM process. For example, Hao *et al.* printed stainless steel and hydroxyapatite composite part which exhibits tensile strength similar to human bone [32]. In addition, Attar *et al.* have successfully printed Ti-TiB composites which has elastic moduli similar to the human bone too [31].

With the above advantages, SLM has a wide impact on industrial manufacturing, not only in prototyping but also in producing functional parts for highly customised applications, such as medical implants and aerospace structures [33, 34]. SLM has been applied to print lightweight structures such as cellular lattice and honeycomb-like structure [35, 36]. In addition, SLM has been employed to manufacture turbine blades, and high temperature applications [21, 37]. Furthermore, many applications in the medical and dental field have adopted SLM to fabricate body prostheses and dental implants. For instance, Wally *et al.* found that Ti6Al4V lattices could enhance the stability of dental implants in elderly and diabetic people with poor bone healing [38]. In addition, drug-delivering implants with releasing micro-channels have been fabricated by the SLM process [39]. Ti-24Nb-4Zr-8Sn parts printed in SLM process has been investigated to reduce the difference of moduli between the implant and surroundings, hence, preventing implant loosening [21]. Therefore, further investigations could advance the applications of SLM.

1.2.2. The benefits and the drawbacks of computational modeling of the SLM process

SLM is a highly complex multi-physics process which involves harnessing optical energy to heat and melt powdered materials in an additive manner [40]. The melting and solidification process of SLM has a majority effect on the eventual mechanical properties of the printed part [41].

Therefore, it is valuable to predict the impacts of the processing parameters on the resulting properties. Furthermore, by investigating the fluid dynamics and thermal gradient of the melt pool, it allows the prediction of defects such as pores, partial-melted powder, residual stresses, and microstructure of the printed part possible. Therefore, several research groups have employed computational modelling to predict the melt pool geometry, defects, and microstructures of selectively laser melted part. For instance, Körner *et al.* [42] developed a numerical tool based on 2D lattice Boltzmann method (LBM) to model local melting and solidification processes of the powder. The model is able to mimic wetting, capillary forces, and the effect of the arbitrary powder bed. Moreover, Leitz *et al.* used numerical models to investigate the impact of powder particle sizes on melt track morphology [43]. The study found that the size and the arrangement of powder have an important impact on the formation of the melt track. Panwisawas *et al.* adopted a computational fluidic dynamics (CFD) model to examine the evolution of porosity in the SLM process [44]. In addition, the microstructure grain growth in the SLM process was also predicted by using a two-dimensional model [45]. Furthermore, Hodge *et al.* applied finite element method (FEM) to investigate the melt pool geometry at the overhanging region [46]. It was found that the volume of the melt pool at the overhang is increased dramatically as compared to the one at the non-overhang location. In summary, computational models can be used to simulate and study the SLM process. Therefore, it can be used to optimise printing parameters, predict defects, and predict the microstructure of the printed part. Last but not least, performing the experiment requires high labour wages and materials expenses, especially for high-cost materials. On a contrary, vary of materials and printing parameters can be tested by employing computational model.

Besides the advantages as shown above, employing computational modelling to simulate the SLM process also leads to some drawbacks. One of the disadvantages of computational modelling is high computational cost and time in developing a multi-physics model. To include one more physic such as the gas-flow inside the chamber, it may need one year or more to develop the model. In addition, the accuracy of the numerical results is dependent on the empirical data obtained from the experiment.

1.3 Objectives

This Ph.D. study aims to achieve four goals. Firstly, a computational model is developed to simulate the melt pool geometry and is validated by SLM experiments. The requirements of this model are to be able to describe the powder bed, the melting, solidification processes, and acting forces such as surface tension, recoil pressure and Marangoni force in the melt pool.

Secondly, the computational model must be able to predict melt pool dynamics of single- and multiple-melt track. By studying the melt pool dynamics, the study aims to propose optimal printing parameters such as laser power, scanning and scanning strategy.

Furthermore, the model is employed to examine the melt pool dynamics in keyhole melt track. As the melt pool dynamics of keyhole-mode melt pool is more complex, further study is required to understand it. Additionally, by investigating the melt pool dynamics, the formation of the defects such as porosity induced in keyhole-mode melt pool would be revealed.

Last but not least, as overhanging structures are unavoidable in SLM, the study also focuses on examining the behaviours of the overhanging melt track under different processing parameters. The model is employed to investigate the discontinuity in the overhanging melt track. Moreover, methods to avoid the discontinuity and related defects will be proposed.

1.4 Research scope and outline of the thesis

In the simulation of SLM, the model should be able to mimic the powder bed deposition process. Furthermore, absorption of the heat source from the laser beam and the heat transfer inside the powder bed must be represented in the model. As melting will happen when the temperature of metal reaches its melting point, the model should therefore be able to simulate the phase-change process from solid to liquid, and from liquid to solid when it undergoes solidification. Additionally, the solid/liquid, solid/gas, and liquid/gas interactions involve in the SLM process, hence, it is necessary to include multiphase-interactions in the model. Last but not least, multiple reflections of laser rays should be modelled. In this research, discrete element method (DEM) was applied to simulate the powder deposition process, while CFD was employed to simulate heat transfer, fluid flows, multi-phase interactions, phase-change process and laser beam interaction inside the powder bed. The outline of the thesis is as follows:

Chapter 1: This chapter gives an overview of AM and the potential of SLM in metal-based AM. The benefits and motivations of computational modelling of the SLM process are also presented.

Chapter 2: This chapter discusses the literature survey of the SLM process, SLM modeling, and the software packages for the simulating the SLM process.

Chapter 3: This chapter details the DEM and CFD methodologies. Firstly, the laser beam was modelled as a simplified heat source applied on the top surface of the powder bed. A ray-tracing model was then employed to simulate the multiple reflections of the laser beam. This chapter also presents the validation of the CFD models.

Chapter 4: This chapter presents the CFD method using a simplified heat source model to study the effect of scanning patterns on the levelness of the melt track in SLM process of SS316L powder.

Chapter 5: This chapter describes the ray-tracing model used to investigate the melt pool dynamics in the keyhole-mode melt pool. Furthermore, this chapter discusses the benefit of the model in predicting the keyhole-induced porosity within the solidified track.

Chapter 6: This chapter discusses the use of the ray-tracing model to investigate discontinuities in the overhanging melt track. The related defects including irregular pores and partially-melted powder are further explained. Suggestions are proposed to avoid discontinuity of the overhanging melt track.

Chapter 7: This final chapter concludes the results and presents future work.

CHAPTER 2: LITERATURE REVIEW

2.1. SLM process and related problems

2.1.1. An overview of the SLM process

SLM is a fabrication technology classified as a PBF system. In the SLM process, a high-energy laser beam is employed to fully melt the powder at the selective region. When one layer of powder has been melted, another layer of powder will be deposited before the melting begins again. Then, by fabricating layer upon layer, 3D objects could be built. In 1999, the first steel powder-based SLM system was launched in Fraunhofer Institute for Laser Technology, Germany [1]. Then, the first commercial SLM ReaLizer 100 machine was introduced in 2005 [1].

Figure 2.1: A schematic overview of the SLM process [16].

The SLM process is depicted in Figure 2.1. A typical SLM machine comprises a powder delivery system, fabrication powder bed system and scanner system. The powder delivery system consists of a spreader and a powder delivery piston. The task of the powder delivery system is to contribute powder to the fabrication powder bed. After one layer is printed, the fabrication piston moves down according to the layer thickness, and then the next layer of powder is deposited by the spreader of the powder delivery system. Next, the powders absorb the heat from the laser beam and are melted. The position of the laser beam is controlled through the scanner system, which includes a system of lenses. The scanner system directs the laser beam to desired points to melt the powder and print the two-dimensional (2D) pattern. Next, the laser beam is either directed to other regions or switched off, while the molten metal cools down and solidifies eventually. Subsequent layers are then deposited and this process repeats until the 3D object is generated.

2.1.2. Physics-related fields in the SLM process

2.1.2.1 Optical system

The optical system in an SLM machine can significantly affect the quality of the printed parts. Figure 2.2 depicts a diagram of the optical system [47] that includes a controlling system, fibre laser, isolator, expander, scanner mirrors, f-theta lens and powder bed. The isolator limits the laser beam to move only in one forward direction. After that, the laser beam goes through the expander increasing the laser beam spot size. The beam is then reflected through the scanning mirrors which are controlled by the controlling system. So when the beam goes through the f-theta lens, the beam is focused on the desired locations.

Figure 2.2: A diagram of the optical system applying in the SLM process [47].

Figure 2.3: Light reflection and absorption [48].

In order to melt the powder, a high-energy laser beam is employed in the SLM process. When an incoming ray of laser beam contacts the powder bed, a portion of the laser energy is absorbed and the rest is reflected as shown in Figure 2.3 [48]. The direction of each laser ray and the power of the reflected ray can be calculated by employing the Fresnel reflection equation and ray-tracing model [49]. Thus, the power absorption of each laser ray in each reflected time can also be computed.

Furthermore, the optical system produces a laser beam containing multiple rays. Furthermore, the laser beam has the distribution of laser intensity as depicted in Figure 2.4. Therefore, each laser ray possesses different laser ray powers and starting points (see Figures 2.4(a, b)), and these rays will reflect multiple times inside the powder bed. In most studies, the laser beam intensity profile was assumed to follow a Gaussian distribution [50, 51]. However, in reality, different optical fibres can produce different laser intensities [52], hence, affecting the laser power distribution. Moreover, the laser beam shape and its intensity can be modified and controlled. For example, Li *et al.* developed an intensity mask with 256 grey levels to convert a near Gaussian intensity beam to a round or square flattop with uniform intensity [53].

Figure 2.4: Schematic of (a) laser ray power distribution, (b) starting point at the focused plane of the laser beam, and (c) powder bed with the focused plane of the laser beam

2.1.2.2 Heat transfer

In the SLM process, the laser beam acts as a thermal heat source and scans at selected areas to melt the powders. The powders and the substrate at the selected areas absorb the heat and transfer the heat to their surroundings. The heat transfer process depends on the thermal properties of the material such as heat capacity and thermal conductivity. Furthermore, the thermal properties of powder material are dissimilar from the bulk material and at different packing densities. For instance, the ratios between the thermal conductivity of powder and thermal conductivity of air

are 3.0, 4.2 and 6.6 for packing densities of 36%, 45% and 55% respectively [16]. Low pack density of the powder bed results in low thermal conductivity due to the high percentage of trapped air. Furthermore during melting and solidification process, the heat loss due to convection, emission, and evaporation also directly influence the heat transfer process [54]. For example, when the temperature of the molten metal reaches the boiling point, a large amount of heat is lost due to the evaporation of the metal.

2.1.2.3 Phase-change

Two phase-change processes, namely melting and solidification, occur during the SLM process [55-57]. On one hand, when the temperature of solid metal reaches the melting point, the solid metal softens and melts. On the contrary, solidification happens when the temperature of liquid metal decreases and reaches the melting point, the liquid metal hardens and solidifies. Furthermore, the material properties are temperature- and phase-dependent [58]. Therefore, during the phase-change processes, material properties such as density, surface tension, thermal conductivity and heat capacity are changed accordingly. For instance, the heat capacity of solid SS316L at 300 K is $502 \text{ Jkg}^{-1}\text{K}^{-1}$, however, its heat capacity in the liquid state is constant at $775 \text{ Jkg}^{-1}\text{K}^{-1}$ [58]. Furthermore, the material properties at the interface are considered as mixed properties [59]. For partially melted powder, the un-melted zone has the material properties of solid state, however, the material properties of liquid state are presented at the melted zone. Thus at the solid-liquid interface, the material properties can be calculated based on the volume fraction of solid/liquid and the material properties at solid/liquid state.

2.1.2.4 Multi-phases interaction

In the SLM process, interactions between phases occur and they are known as multi-phase interactions. Figure 2.5 depicts the different phases of materials found in the SLM process including the solid phase of powders, the liquid phase of the melt pool, and the gas phase of inert gas. Matthews *et al.* performed high speed imaging capture and found that the solid particles can be pulled into the molten melt pool signifying an interaction between the two phases [60]. Furthermore, the inert gas flow also affects the spattering of powder particles. The study found that the transport of heavier and larger spattering particles is raised by increasing the gas velocity [61].

Figure 2.5: A schematic of multi-phase interaction in the SLM process

2.1.2.5 Fluid dynamics

Fluid dynamics play a significant role in understanding the melt pool characteristics [41, 62]. The studies of melt pool dynamics provide insights to the formation of melt track [63] and defects such as porosities, balling and humping [64]. Furthermore, printing parameters including laser power, scanning speed, hatch spacing, layer thickness of powder and scanning strategy directly

affect the melt pool dynamics. For instance, at low energy density due to insufficient heat source, the melt track tends to break into droplets instead of spreading uniformly, hence, forming balling melt track [65]. Therefore, by investigating the melt pool dynamics, the printing parameters can be optimized. Moreover, the melt pool dynamics also affects melt track morphology. In addition, the generation of defects such as pores and partially melted powders can be revealed by investigating the dynamics of the melt pool. For instant, the formation of pores can be understood by studying the velocity field of the melt pool [66].

2.1.2.6 Powder and substrate

Previous study has shown that different powder sizes lead to variation of the melt track width [43]. Moreover, the powder size and powder density have a critical impact on the density of the printed part [57]. The study found that when the powder bed has a higher packing density, the melt track will be more defined. Table 2.1 lists the powder sizes of several materials employed in SLM. As can be seen, a variety of sizes of SS316L were used in SLM. The powder can be coarse at diameters from 35 to 55 μm [35], at medium sizes from 20 to 53 μm , or finer at 15 to 45 μm [67]. Besides processing parameters such as laser power and scanning speed, the packing density of the powder bed also influences on the melt track morphology, where a uniform melt track could easily be formed at high packing density [57]. Therefore, to increase the packing density of the powder, a mixture of powder sizes was proposed [68]. As proven, previous study has shown that the density of bimodal mixtures was always higher as compared to mono-sized powder [69]. Therefore, Wang *et al.* were used the powder mixtures to perform SLM printing [70]. The powder mixtures were used containing different size classes ranges from 15 to 30 μm . By employing 50 % of the smallest size class, a small mean diameter of the powder bed of 17.11

μm was generated. Next, the properties of the printed part are also dependent on the pre-heating of the substrate. It is possible to use pre-heating substrate to reduce the cooling rate, hence, preventing cracking during the solidification [71]. For instance, in the fabrication of Ni625, the substrate was pre-heated to 150 °C and 300 °C, and at 300 °C, large cracks were alleviated [72]. Moreover, residual stress was recorded to be 160 ± 25 MPa if the substrate was pre-heated to 300 °C, while the residual stress of the part printed under ambient temperature was 396 ± 23 MPa [72].

Table 2.1: Powder sizes of different materials.

Material	Powder distribution	Powder size (μm)	Reference
Ti-6Al-4V	Gaussian	45 – 115	[42]
AlSi10Mg	–	20 – 60	[73]
Nickel-based superalloy	Gaussian	15 – 55	[74]
SS316L	Gaussian	17 – 37	[75]
SS316L	Gaussian	45 ± 10	[35]

2.1.2.7 Chemical reactions

In order to avoid oxidation of metal during the SLM process, the chamber needs to be filled with the inert gas such as argon or nitrogen. Moreover, the lens, substrate, and recorder are cleaned carefully to avoid unwanted chemical reactions. Li *et al.* found that during the fabrication of Al-12Si, Al reacts with the moistures at the skin of powder surface to form Al oxide and Al hydroxide [76]. Therefore, by removing the moisture powder surface, dried Al-12Si powder was employed to enhance the density of the printed part. Besides, Attar *et al.* found that due to the

chemical reaction, the mechanical properties of Ti-TiB composites is increased [77]. As the TiB₂ particles in irregular shape react with pure Ti to shape needle-shape titanium monoboride (TiB) particles. Due to the existence of B, Ti grains are significantly refined, enhancing the microhardness, yield stress and compressive strength.

2.1.2.8 Parameters impact on SLM process

There are around 130 parameters that could influence the quality of the printed part [16]. The parameters such as laser power, beam size, layer thickness and scanning speed influence the melt track morphology and the melt pool geometry. Gong *et al.* studied the effect of laser power and scanning speed on the melt pool geometry. The melt pool was in conduction-mode at low laser power or high scanning speed, however, a keyhole-mode melt pool was formed when a high laser power or a low scanning speed was applied [78]. In addition, Zhao *et al.* studied the relative density of printed parts by employing different laser powers and scanning speeds [79]. It found that the relative density was decreased by increasing the scanning speed or reducing the laser power. By applying same scanning speed of 550mm/s, the density of the carbon/AlSi10Mg printed part was improved from 90% at the laser power of 240 W to 97% at the laser power of 300 W. In addition, by employing same laser power of 50 W and scanning speed of 100 mm/s, the melt track was continuous at a low layer thickness of 50 μm , however, balling happened at the layer thickness of 200 μm [80]. Furthermore, high layer thickness leads to porous structure of the printed part [81]. Qiu *et al.* printed Ti6Al4V samples and found that the area fraction of porosity jumped from 0.09% at the layer thickness of 20 μm to 10.68% at the layer thickness of 100 μm . Additionally, the laser beam size also directly affects the printed part. According to Aggarwal *et al.*, a shallow melt pool was formed at the beam radius of 47.9 μm , while a deep

penetration appeared by employing a beam radius of 25 μm [82]. Nevertheless, processing parameters bring a major effect on the melt pool dynamics which influence significantly on the properties of the printed part including porosity, surface roughness, and microstructure [63, 81]. For instant, Tan *et al.* explained the formation of spherical and elliptical pores at the bottom of the keyhole by employing computational model [66]. Under high energy density, a deep keyhole was penetrated and collapsed. Then, the molten metal encircled and trapped the gas bubbles into the melt pool, forming pores at the bottom of the keyhole. Furthermore, the surface roughness is also affected due to the melt track morphology [83, 84]. For instant, balling melt track resulted in high surface roughness of as-fabricated SLM part. In addition, the molten metal was also exhibited thermal gradient inside the melt pool, hence, directly affecting the evolution of the grain growth resulting in the final microstructure [85]. For example, Liu *et al.* applied a much higher cooling rate on top of a melt pool as compared to the one at the bottom [85]. It led to the formation of gradient microstructure in the AlSi10Mg as-fabricated part, and at the surface, Si particles were distributed evenly, and finer dendrites were formed. As a result, the surface hardness of printed part was improved.

2.1.3. Mechanical properties of SLM part

Density, hardness, tensile strength, residual stress, and surface roughness are among the most important characteristics of 3D printed metallic parts [46]. The processing parameters directly affect the density of the printed part. According to Zhang *et al.*, under the same laser power of 200 W, a high density part of 99.3% was produced at the scanning speed of 550 mm/s, however, a low density of 98.5% was formed at the scanning speed of 800 mm/s [86]. Moreover, different scanning speeds lead to different values of the Vickers hardness, where lower scanning speed

produced the printed part with higher Vickers hardness [86]. In addition, Montero-Sistiaga *et al.* examined the effect of high laser power on the mechanical properties of the printed part [87]. The study found that high laser power produced as-printed part with yield tensile strength was comparable with the part employed low laser power. However, low elongation and low ultimate tensile strength were generated. Fortunately, the mechanical properties were notable surpassed by employed hot isostatic pressing (HIP) post processing [87]. Moreover, as the SLM process experienced rapid melting, cooling and re-melting, it induced residual stress leading to microcrack and distortion of the as-fabricated part [88]. Therefore, many studies have investigated residual stress in the SLM process [88, 89]. By applied different scanning strategies, it produced different residual stress in the printed part [90]. For instant, by preheating the powder bed to 100 °C, chessboard scanning strategy produced residual stress of 179 MPa, while the 90° alternating gave a printed part with the residual stress of 100 MPa. Furthermore, surface roughness is also one of the criteria to examine the SLM printed part. Sing *et al.* illustrated the surface roughness at the top and the side of the Titanium-tantalum (TiTa) alloy as-printed part [91]. The study found that by employing high energy density, surface roughness at the top surface was reduced. As lager melt pool was formed by applying high energy density, then, it enhanced the overlap in between the melt track. As a result, the surface finish is improved. Additionally, surface roughness has been paid greatly attention in overhanging printing [92]. Where the melt track was printed fully or partially on top of a thick layer of powder, it called overhanging printing. As SLM process supports to print complex geometry such as latticed structure, or honeycomb, hence, overhanging printing are unavoidable. In addition, the formation of dross in overhanging printing is commonly to be found, and it affects the surface roughness of the overhanging as-

printed part [93]. Covarrubias *et al.* investigated that the roughness of downward surface is typically higher than the one of top surface in overhanging printing [94].

Additionally, the SLM process can be used with different metallic powders such as stainless steel, titanium alloys, and aluminium alloys. Table 2.2 compares the mechanical properties of parts made from Ti-6Al-4V [20] and AlSi10Mg [95] that are produced by SLM and the conventional casting. It shows that SLM can produce parts which possess very good mechanical properties. Furthermore, it can be seen that Young's moduli of parts produced by SLM are close to that produced by the conventional method.

Table 2.2: Mechanical properties of Ti-6Al-4V and AlSi10Mg in SLM and conventional casting.

Material	Fabricating method	Young's modulus E (GPa)	Tensile strength (MPa)	Maximum elongation ϵ_{break} (%)
Ti-6Al-4V [7]	SLM	109.2 ± 3.1	1267 ± 5	7.28 ± 1.12
	Conventional casting	120.2 ± 1.9	1006 ± 10	18.37 ± 0.88
AlSi10Mg [26]	SLM (<i>x-y</i> direction)	68 ± 3	391 ± 6	5.55 ± 0.4
	Conventional Casting	71	300 – 317	2.5 – 3.5

2.1.4. Limitations of the SLM process

As previously discussed, there are many advantages of using SLM in metal fabrication such as reducing the production time and ability to fabricate high complex intricate functional parts. However, SLM has its drawbacks too. First of all, SLM contains many random factors that bring challenges to fully understand the process. For instance, the powder bed distribution is non-uniform across all layers. Additionally, powder was spattered during the printing process exacerbating the uniformity of the powder bed [47]. As a result, surrounding melt tracks would be affected in terms of their morphologies and the melt pool geometry. Till date, it is still a challenge to maintain the consistency of powder distribution, temperature distribution, and melt pool geometry throughout the layers. Moreover, in the SLM process, a high-energy laser beam is employed to supply heat to the powder bed over a very short duration at specific locations. This causes a large thermal gradient which in turn results in thermal stresses [20]. Additionally, the thermal gradient is also affected by scanning strategies, which affects the microstructure of the as-printed part [96, 97]. In other words, different scanning strategies produced different microstructures of the printed part and hence varies of the inherent mechanical properties. Additionally, porosity (1 to 2%) also exists in the printed parts which may cause critical problems in applications where high strength and fatigue resistance are required [84]. To solve these problems, it was reported that re-melting a layer before printing the next is able to improve the quality of the printed parts [84]. As reported, the selectively laser melted as-printed part without re-melting exhibited 0.77% of porosity. However, the percentage of porosity was reduced to 0.036% by applying re-melting using selected processing parameters. Furthermore, geometrical inaccuracy also happened in SLM, especially, in overhanging structures [93, 98, 99]. For instance,

serious warping could appear in the overhanging printed part by employing low inclined angle of 25° [70].

2.2. Review of computational methodologies for the SLM process

In the SLM process, to achieve functional parts meeting the quality standards, suitable processing parameters are typically chosen by trial and error experiments, which could be time consuming and expensive. Accordingly, many works have employed simulation techniques to investigate the AM process. Through various simulation methods, one may gain deep insights into the physical mechanisms underlying the complex phenomena during the SLM process, such as the melt pool dynamics, thermal evolution, growth of microstructure, etc. This section discusses the different computational methods for different approaches including particle interactions, heat transfer and flow field prediction.

2.2.1. Particle interactions

To perform the particle interactions in the powder bed, DEM is an efficient practice which was employed by many studies. DEM is a numerical method generally employed for modelling a large number of small particles. The motion of particles is computed by applying Newton's equations of motion, and the method is closely related to molecular dynamics [40] and each solid grain or particle is treated as one element, hence, reducing computational costs. In engineering problems, DEM is an effective method in solving granular or discontinuous materials, for instance, granular flows, powder mechanics and rock mechanics [100-102]. Naturally, DEM is a strong candidate to simulate the powder bed. The advantage of the DEM is that the particles could be simulated in different sizes and materials [103, 104]. For instance, Gu *et al.* simulated

powder bed deposition of Inconel 718 in which the materials were different in sizes as depicted in Figure 2.6 [104]. In addition, the deposition of the powder bed containing two different materials including WC and Inconel 718 was simulated [104].

Figure 2.6: Simulated powder bed morphology of Inconel 718 powder particles with average diameter of (a) 15 μm , (b) 25 μm , (c) 35 μm , and (d) 45 μm [104].

2.2.2. Heat transfer

Different methods have been employed to simulate the heat transfer in the SLM process. One of the most common method has been adopted to mimic the heat transferring process in the printing of the selective laser melted part is finite element method (FEM). FEM is applied to approximate solutions of partial differential equations using numerical techniques. In this method, a complex and large problem is divided into simpler and smaller parts called finite elements. Each element

consists of nodes (for example, three nodes for triangular element and four nodes for rectangular elements) which are coordinate locations in space where the degrees of freedom (DOFs) are defined. In each element, the physical values such as force and displacement can be modelled by simple equations. Then these simple equations can be assembled to become a large system of equations to model the entire problem. The approximate solutions are determined by an associated error function. FEM was applied in part-scale SLM modelling. A part of the SLM process includes heat transfer and solid mechanics. Hodge *et al.* [46] presented a continuum model using Diablo code to determine the melt pool geometry. The simulated melt pool shape is close to that of Gusarov's work [105] as shown in Figure 2.7.

Figure 2.7: Melt pool geometry simulated by (a) Gusarov [105] and (b) employing multi-physics finite element code Diablo [46]. The contour represents the melt pool boundary.

Although the FEM model is relatively simple, it provides sufficient insight to where the melting will occur and the stresses are. In addition, FEM could be applied in both mesoscopic and macroscopic model [106-108]. In Zhang's work, the model could predict the temperature distribution of complex geometrical part during the SLM process at the macroscale [106]. The study also employed a refining and de-refining mesh adaption to reduce the computational cost. In addition, FEM is suitable to reveal the thermal stress and mechanical properties of the printed part. For example, Ahmadi *et al.* employed a FEM model to predict the mechanical properties of

the printed samples [107]. The study found that the mechanical properties of as-printed samples such as stress and strain are closely related to the modelling result. However, the FEM model is unable to represent discrete powders. In addition, the molten flow in the melt pool cannot be mimicked by employing the FEM.

Figure 2.8: Temperature distribution of the powder bed on 4th, 23rd, 30th and 40th layer [109].

Apart from FEM, DEM has also been employed to model the heat transfer in the powder bed. Figure 2.8 depicts temperature distribution at different layers in which the heat is transferred from high (red) to low temperature (blue) [109].

Furthermore, the heat transfer during the melting and solidification process can be adequately simulated by employing the CFD model. Different methods including Lattice Boltzmann method (LBM), volume of fluid (VOF) method and Arbitrary Lagrangian-Euler (ALE) have been employed to develop the CFD model to simulate the heat transfer and melt pool dynamics in the SLM process. The details of these methods are described in the section 2.2.3.

2.2.3. Flow field prediction

Lattice Boltzmann method (LBM), volume of fluid (VOF) method and Arbitrary Lagrangian-Euler (ALE) are the three common practices which have been adopted in simulating the flow field in the SLM melting and solidification process. The following sub-sections present in detail about each method.

2.2.3.1. Lattice Boltzmann method

Lattice Boltzmann method (LBM) is a technique to solve various fluid flow problems by employing pseudo-particles that are moving and interacting with one another following the Boltzmann equations [110]. The LBM was employed to simulate heat transfer, phase-change, and multiphase interaction in different applications [111, 112]. In LBM, the computational domain is divided into sub-domains which are called cells. Each cell has a probability to find a

particle or fluid at a particular time, position and velocity. Several groups have adopted the LBM to gain insights into the SLM process.

Table 2.3: Material properties of Ti–6Al–4V in experiments and LBM simulations [57].

Material properties	Experimental value	LBM (*)	Relevant scale
Density at liquid state	4000 kg/m ³	1.0	$\rho^* = \rho \frac{\Delta x^3}{\Delta m}$
Viscosity	0.005 Pas	0.011	$\nu^* = \nu \frac{\Delta t}{\Delta x^2}$
Surface tension	1.65 N/m	0.15	$\sigma^* = \sigma \frac{\Delta x^2}{\Delta m}$

Figure 2.9: Melt pool geometry at different particle packing densities from 39% to 74% [57].

Alexander *et al.* [113] employed a 2D free surface LBM to solve the hydrodynamics and thermodynamics of molten powder. The model considered the effects of evaporation due to mass losses and recoil pressure on the melt pool. The study shows that the 2D LBM model is able to simulate and produce melt pool geometries in a close agreement with the experiment. In addition, Körner *et al.* [57] developed a numerical tool based on the LBM to simulate powder melting and solidification processes at powder-scale in 2D. In the numerical simulations, the material parameters were expressed in dimensionless form as tabulated in Table 2.3. The study shows that powder density has a significant influence on the melt pool characteristics. Accordingly, the melt pool geometry becomes more uniform at high powder packing density (see Figure 2.9). The numerical investigation was also conducted on successive assembling in layers. Figure 2.10 shows the quality of the walls printed with different layer thicknesses. It shows that the quality of the walls sinks obviously as the layer thickness increases [42]. In the Figs 2.9 and 2.10, apart from LBM, the rain model using for random deposition of particles has been applied [57].

Figure 2.10: Printed walls at the layer thickness of (a) 150 μm , (b) 100 μm , (c) 70 μm , (d) 50 μm and (e) 35 μm [42].

2.2.3.2. Arbitrary Lagrangian-Euler method

Arbitrary Lagrangian-Euler (ALE) is a numerical technique to solve fluid dynamics and nonlinear solid mechanics using FEM and finite volume method (VFM) [114]. ALE3D, developed by Lawrence Livermore National Laboratory, is a 2D and 3D multi-physics numerical simulation software tool using the ALE method. Furthermore, the software is able to handle many hybrid finite element and finite volume problems such as heat conduction, chemical kinetics, incompressible flow, and multi-phase flow with long to short time-scale simulation. Khairallah *et al.* [75] made use of the software to simulate the melt pool track in the powder scale. It was found that with surface tension, heat will transfer faster while the melt track will cool down sooner as shown in Figure 2.11. Furthermore, the simulation results of the melt pool characteristics were well-aligned with the experimental work (see Figure 2.12). In their work, the influences of temperature and scanning velocity on the melt pool track were also studied. At low speed, the melt surface is smoother and formation of residual pores is decreased. In addition, the simulation results proved that recoil pressure and Marangoni convection have significant effect on the generation of melt track, pores and material spattering [63]. The effects of laser intensity profiles on single-track macrostructure and microstructures were also explored [115]. The study found that the grain morphology can be customized by varying the laser beam intensity profile while employing a constant laser power and scanning speed.

Figure 2.11: Morphology of melt track (a) with and (b) without surface tension [75].

Figure 2.12: The melt pool height, depth and width are (a) 26, 30 and 75 μm in the experiment respectively, and (b) 26, 20 and 72 μm in the simulation respectively [75].

2.2.3.3. Volume of fluid method

Volume of fluid method (VOF) is employed to track free surfaces such as the fluid-gas interface or liquid-liquid interface [116]. Furthermore, VOF model has been adopted in the modelling and simulation of the SLM process [41, 117]. In the fabrication of a selectively laser melted part, the

powder is melted, cooled, solidified and subsequently fused together. The process can be adequately modelled by a CFD model using the VOF method to capture the gas-metal interface as exemplified in Figure 2.13 [62]. As depicted in the Figure 2.13, Gürtler *et al.* made use of a CFD toolbox known as OpenFOAM® (Open Field Operation And Manipulation) to model and simulate the melting process [41]. The CFD model was improved by adding spacing between the solid phase to represent the powder. By applying the laser heat source on the top surface of the powder bed, the simulation of the melting and solidification process of powder bed was performed.

Figure 2.13: Simulated single laser scan line at 300 μs [41].

2.2.4. Combination of particle interactions, heat transfer and flow field prediction

The coupling of CFD-DEM method is able to simulate a system containing both flow (liquid or gas) and solids or particles [118]. The motions of solids or particles are calculated by the DEM model where Newton's second law of motions is applied. Besides, the flow of fluid liquid is computed by solving the conservation of mass, momentum and energy equations via the CFD model. The interaction between the flow and the solids/particles described by CFD and DEM is executed using Newton's third law. The coupling of CFD-DEM method has been used in other field to simulate the model containing both air and particles as shown in Figure 2.14 [119]. In the model, the temperature of particles was kept constant (600 K) while the air enters from below at a temperature of 263 K. Then, the velocity of airflow and the heat flux of the particles were computed by solving CFD-DEM equations. However based on my research, the interactions of solid-liquid-gas phases have not been considered in the current SLM simulation. As it is a challenging task, it needs much more knowledge, time, and resources to develop a CFD-DEM solver which can simulate the movement of particles during the melting and solidification process, for instance, the solid particles are pulling into the melt pool. Yet, this method opens the idea in simulating the motions of powder particles during the melting process in SLM.

Figure 2.14: CFD-DEM velocity, temperature and heat flux simulations where the temperature of particles was kept constant (600 K) while the air enters from below at a temperature of 263 K [119].

2.2.5. Discussions

In the simulation of the SLM process, two main steps need to perform. Firstly, the model should be able to imitate the deposition of the powder. Secondly, the model can offer the capability in simulating the melting/solidification process. The deposition of the powder bed can be done by applying the model using DEM. Unfortunately, the DEM method is unable to model the melting process which is a critical phenomenon in the SLM printing. On the contrary, the CFD method is unable to model the discrete powders but yet adequately simulate the melting/solidification process. Therefore, in order to model both the discrete powders and the melting process, it is essential to make use of the coupling of the CFD-DEM method. Among the CFD approaches, several simulation works making use of ALE have been published, however, the software is not publicly available commercially or academically. The LBM can also simulate the melting/solidification process, with some current publishes are able to simulate the surface

morphology such as humping closely to the experiment [120]. However due to the complexity of the method and lack of resources in the starting point of the project, LBM was not chosen. Whereas, the VOF method is more popular in references and software packages. Therefore, the VOF method was chosen to develop the CFD model.

2.3. Software packages using for SLM simulation

2.3.1. Software packages for DEM model

Two common software packages named ANSYS EDEM and LIGGGHTS[®] can be employed to simulate the particle interactions.

2.3.1.1. ANSYS EDEM

EDEM is a software package based on advanced DEM from DEM Solutions Ltd., which is a global leading software company providing solutions for solving bulk material flow [121]. The software is able to simulate and analyse the behaviour of individual particles, integrating particles, fluid, and machine dynamics. EDEM is employed in a variety of industrial problems such as agriculture, chemical processing and pharmaceuticals [122, 123].

EDEM is able to work in ANSYS Fluent environments by coupling EDEM and CFD model. By adding discrete particles to the continuum model, EDEM CFD coupling has the capability to solve particle-fluid flows as well as solid-liquid phase. To serve different purposes, users can customize the source code to decide how EDEM and ANSYS Fluent work together.

2.3.1.2. LIGGGHTS®

LIGGGHTS® (LAMMPS Improved General Granular-Granular Heat Transfer Simulation) is an open-source DEM particle simulation software based on LAMMPS [124]. Some advantages of LIGGGHTS® are open-source where one can access to the algorithms freely and its ability to be implemented in CFDEM® by coupling with a CFD model. The DEM model built in LIGGGHTS® can also be easily modified as an open-source code software. Different research groups have employed LIGGGHTS® to perform the deposition of powder bed in the SLM process [43, 125]. Leitz *et al.* generated molybdenum powder beds with a layer thickness of 20 and 40 µm for further investigating the effect of powder bed characteristics on the melt track morphology [43]. In addition, the melt pool dynamics of the keyhole was performed employing Ti-6Al-4V powder bed which was generated in LIGGGHTS® [125].

2.3.2. **Software packages for CFD model using VOF method**

Various CFD software packages using VOF method have been employed to simulate the SLM process, including ANSYS FLUENT, FLOW-3D, and OpenFOAM®.

2.3.2.1. ANSYS FLUENT

ANSYS FLUENT, a commercial CFD software, is able to solve flow, turbulence, heat transfer and reactions for industrial applications [126]. It offers high performance computing to solve complex and large model efficiently and cost-effectively. It was employed to simulate melt pool geometry and velocity field in the SLM process using point exposure and continuous exposure scanning strategies [127]. In addition, ANSYS FLUENT was also adopted to simulate temperature field and grain growth of SLM of AlN/AlSi10Mg composite [128]. The study

investigated that the cooling rate has a major influence on the morphology of the microstructure. As reported, directional columnar cellular appeared at the region near the substrate due to the high cooling rate. However, as the temperature of the substrate is increased in the following layers, it enhanced the formation of other microstructures such as refined cellular and coarse cellular.

2.3.2.2. Flow-3D

Flow-3D is a commercial software [129] which has been widely adopted to simulate the PBF process such as SLM and EBM. Pei *et al.* have investigated the effect of laser power, scanning speed and hatch spacing on the thermodynamics of the molten pool of the SLM process of AlSi10Mg powder [130]. The study found that the instability of the melt track happens at high scanning speed. Furthermore, Yan *et al.* also used FLOW-3D software to perform the CFD simulation to optimize the hatch spacing in PBF process [131]. The study found that the hatch spacing should not be larger than the width of the re-melted region within the substrate.

2.3.2.3. OpenFOAM®

OpenFOAM® is an open source software package employed in many different fields of engineering and science [132]. OpenFOAM® provides solutions to simulate different problems such as water flow, heat transfer, multi-phase interaction and phase-change. As a result, OpenFOAM® was employed to simulate the SLM process [41]. The formation of pores has been investigated by using the CFD model developed in OpenFOAM® software [44]. It was found that the pores will change from near-spherical to elongated shape as the scanning speed increases.

This happened due to the exertion of the forces including vapour pressure and thermal capillary forces on the metallic/gaseous interface. Furthermore, Panwisawas *et al.* have investigated thermal fluid flow in the powder bed with different layer thicknesses and scanning speeds [59]. In addition, the study also examined the effect of thermal history on the grain growth. In the microstructure of as-printed part, the columnar grains were dominant due to high thermal gradient in the SLM process. This prediction had a good agreement with the electron backscattered diffraction data.

2.3.3. Software packages for the coupling of CFD-DEM

Several software packages, such as ANSYS EDEM coupled with ANSYS Fluent, MFiX, and CFDEM[®] can be employed to solve CFD-DEM problems. In this report, we would elaborate on the latter two which are open source.

2.3.3.1. MFiX

MFiX is an open source multi-phase flow solver [133]. The software consists of four models that treat the gas and solid phase differently. Listed in Table 2.4 are the four models which are MFiX-TFM (two-fluid model), MFiX-PIC (multi-phase particle in cell), MFiX-DEM and MFiX-Hybrid (Eulerian-Lagrange-Eulerian). The MFiX-TFM and MFiX-DEM models are able to solve momentum equations, energy equations, chemical reactions, and Cartesian cut-cell which is employed to simulate the curve boundary in the Navier–Stokes equation [134]. By applying curved boundary, the interface such as liquid/liquid interface or liquid/gas interface can be sharpened. Regarding to MFiX-PIC and MFiX-Hybrid, momentum equations and Cartesian cut-cell are available.

Table 2.4: Basic models in MFiX and their features [133].

	MFiX-TFM	MFiX-PIC	MFiX-DEM	MFiX-Hybrid
Momentum equations	●	●	●	○
Energy equations	●	—	●	—
Chemical equations	●	—	●	—
Cartesian cut-cell	●	○	○	○
● implemented and fully tested ○ implemented with limited testing				

2.3.3.2. CFDEM[®]

CFDEM[®] is an open source CFD-DEM engine [135]. It provides a platform to couple the DEM engine by LIGGGHTS[®] to a CFD engine by OpenFOAM[®] in order to solve large-scale problems. Using CFDEM[®], the solid powder in the SLM process can be modelled by DEM using LIGGGHTS[®], while the melt track can be addressed by the CFD method using OpenFOAM[®]. Recently, the coupling of CFD and DEM model has been successfully employed in the simulation of the SLM process [136]. The study used a sharp surface capturing technique (iso-Advector) to reconstruct the interface between different phases. In addition, the solidified metallic/gaseous interface was assumed as a solid boundary for depositing of the next layer. Figure 2.15 shows the deposition of metal powder on top of the solidified surface.

Figure 2.15: Powder bed deposition on a solidified surface using CFD-DEM model [136].

2.3.4. Discussions

The chosen software packages should be able to simulate the powder deposition using DEM model, and the melting/solidification process using CFD model. In order to fully simulate the SLM process from powder deposition to melting and solidification process, it requires the possibility of coupling the DEM and CFD models for the CFD-DEM model. After much testing and deliberation, it was decided that LIGGGHTS[®] (DEM), an open-source software package, is used for modelling the deposition of powder. Furthermore, OpenFOAM[®] (CFD), a CFD open-source code which is able to coupling with LIGGGHTS[®], was chosen as a platform for the simulation of heat transfer, melting and solidification process. The open-source software packages were employed due to the free access. Moreover, the main focus in the study is to make use of the CFD model to investigate the melt pool dynamics and the formation of the melt track in the SLM process. It is because the CFD model is able to simulate the melt pool dynamics where the formation of defects such as pores and partially melted powder can be revealed.

However, in the current CFD model, the powder is unmovable during the printing process. To improve the simulation model, the motions of powder during the printing process should be included. Therefore in the future study, CFDEM[®] (CFD-DEM) will be employed to simulate the movement of powder and the melting process concurrently

2.4. Summary

SLM is a highly complex multi-physics process, including heat transfer, multi-phase interactions, phase-change, and laser-material interactions. During the printing process, the powder is firstly deposited on the substrate, then a high power of laser beam is employed to fully melt the powder particles. In the numerical modelling, DEM model was adopted to imitate the deposition of powder, and the CFD model is employed to simulate the melting/solidification process. The DEM model developed using LIGGGHTS[®] and the CFD model developed using OpenFOAM[®] were employed to simulate the SLM process. Currently, the DEM and the CFD models are coupled manually to mimic the SLM process. To simulate the motions of particles during the melting process, it is essential to make use of the coupling of the CFD-DEM method which can be performed in the platform of CFDEM[®].

CHAPTER 3: COMPUTATIONAL METHODOLOGIES AND MODEL VALIDATION

This chapter presents the computational methodologies and the validation of the computational model. In order to simulate the SLM process, different models were employed to imitate closely to the SLM experiment. The DEM model was adopted to simulate the deposition of the powder, while the CFD model was used to model the melting and solidification phenomenon in the SLM process. The laser beam was modelled as a simplified heat source applied on the top surface of the powder bed to simulate conduction-mode melt pool and medium-deep keyhole-mode melt pool. The multiple reflections of the laser beam were also modelled by employing the ray-tracing model. The model was employed to simulate well-deep keyhole-mode melt pool. Furthermore, both of the simplified heat source model and ray-tracing model were validated by comparing the melt pool geometry of the simulation to the one of the experiment.

3.1. DEM model

3.1.1. Methodology

In this work, the DEM model was employed to simulate the deposition of the powder. In the model, Newton's second law is used to calculate the position of the powder particles. From the Newton's second law, the change of position against time of an i^{th} particle can be determined by [40, 119]

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i^{total}, \quad (3.1)$$

where m_i is the mass of the particle i , r_i is its position, and F_i^{total} is the total force on the particle i .

In the DEM model, both frictional and gravitational force make up the total force which is calculated as

$$F_i^{total} = F_i^{fric} + F_i^{gra}, \quad (3.2)$$

where F_i^{fric} and F_i^{gra} are the frictional and gravitational forces on the particle i respectively.

When the particles do not overlap, the only active force is the gravitational force, which is described as [40]

$$F_i^{gra} = -m_i g \hat{z}, \quad (3.3)$$

where m_i represents the particle mass, g is gravity and $\hat{z}$ is the unit direction in the z -axis.

The particles overlap when the distance r_d between two particles of radius R_i and R_j is less than their contact distance $d = R_i + R_j$ as shown in Figure 3.1. In this case, besides the gravitational forces, the friction forces are also exerted on the particles.

Figure 3.1: Schematic of the overlapping particles

The friction force between two granular particles is described by [137]

$$F_i^{fric} = (k_n \delta_{n_{ij}} - \gamma_n v_{n_{ij}}) - (k_t \delta_{t_{ij}} - \gamma_t v_{t_{ij}}), \quad (3.4)$$

where, $\delta_{n_{ij}} = d - r_d$ is the overlap distance between two particles, k_n and k_t are the elastic constant for normal and tangential contact respectively, and γ_n and γ_t denote the viscoelastic damping constant for normal and tangential contact respectively. $\delta_{t_{ij}}$ is the tangential displacement vector between two spherical particles, and $v_{n_{ij}}$ and $v_{t_{ij}}$ represent the normal and tangential component of the relative velocity of the two particles respectively. In this study, sliding friction was considered to mimic the sliding interaction of particles. However, rolling friction has not been presented yet, and it lessens the accuracy of the model. To improve its accuracy, the rolling force will be included in the future study.

The friction force for tangential contact is computed as [137]

$$F_t = k_t \delta_{t_{ij}} - \gamma_t v_{t_{ij}}, \quad (3.5)$$

where F_t is the friction force for tangential contact. And the friction force for normal contact is described as [137]

$$F_n = k_n \delta_{n_{ij}} - \gamma_n \nu_{n_{ij}}, \quad (3.6)$$

where F_n is the friction force for normal contact.

The requirement of friction force for normal contact and tangential contact is

$$F_t \leq \mu_f F_n, \quad (3.7)$$

where μ_f is the coefficient of friction.

From the material properties, k_n , γ_n , k_t , and γ_t are calculated as [138]

$$k_n = \frac{4}{3} Y^* \sqrt{R^* \delta_n}, \quad (3.8)$$

$$\gamma_n = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*}, \quad (3.9)$$

$$k_t = 8G^* \sqrt{R^* \delta_n}, \quad (3.10)$$

$$\gamma_t = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m^*}, \quad (3.11)$$

where

$$S_n = 2Y^* \sqrt{R^* \delta_n}, \quad (3.12)$$

$$S_t = 8G^* \sqrt{R^* \delta_n}, \quad (3.13)$$

$$\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}, \quad (3.14)$$

and

$$\frac{1}{Y^*} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}, \quad (3.15)$$

$$\frac{1}{G^*} = \frac{2(2-\nu_i)(1+\nu_i)}{Y_i} + \frac{2(2-\nu_j)(1+\nu_j)}{Y_j}, \quad (3.16)$$

$$\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}, \quad (3.17)$$

$$\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}, \quad (3.18)$$

where Y is the Young's modulus, ν is the Poisson's ratio, G is shear modulus and e is the coefficient of restitution.

The simulation domain is bounded by frictional walls not limited to any geometry. The interaction between the particles and walls is calculated by the same Eqns. (3.4) and (3.17) used to compute the interaction of two particles where the wall has an infinite radius. The geometries of the frictional walls will be imported as an ASCII STL file or Visualization Toolkit (VTK) file to form a triangular surface mesh for the DEM simulation. The program will calculate the curvature of the mesh, hence, the interaction of the particles and the mesh wall can be computed. Furthermore, the simulation platform also supports for movable objects of any geometry whose parameters such as velocity and moving direction can be set.

In the current DEM model, the hydrodynamic force between the particles such as the van-der-Waals force has not considered yet. The contact force and the gravitational force are stronger than the van-der-Waals force, directly driving the motions of the powder particles. In fact, the model will be more accurate when the hydrodynamic forces and the interaction forces between

particles (not touch each other) are considered. However, with the current forces including the gravitational force and the contact force, the free surface of the powder bed can be simulated. In addition currently, generating a free surface morphology of powder bed is the main purpose of employing DEM model. For further investigating the influence of particles sizes, shapes and motions, the van-der-Waals force and the rolling friction force should be considered in the coupled CFD-DEM model to achieve high accuracy in the simulation results.

3.1.2. Simulation parameters and material properties

In the simulation, SS316L was employed. The simulation parameters and the material properties used in the DEM model are listed in Table 3.1. The properties of solid phase such as density, Poisson's ratio, friction coefficient, restitution coefficient, thermal conductivity, and heat capacity are kept constant in this simulation. A small Young's modulus and coefficient of restitution were applied to reduce the computational cost in the DEM model. If the DEM model uses a Young's modulus close to the experimental value, the time-step for DEM simulation would have to be quite small (about 0.1 ns) to ensure numerical stability. With the sacrifice of a little accuracy, the small values of Young's modulus and coefficient of restitution can significantly improve the computational efficiency, while the final configuration of simulated powder bed is still analogous to the real experiment. For example, Nan *et al.* adopted a Young's modulus of 2.2 GPa with the time-step of 10^{-8} s to simulate the SS316L powder bed [139]. Thus in this work, a Young's modulus of 1.1 GPa and coefficient of restitution of 0.3 were employed to lower the time-step to 10^{-7} s. In the model, the particles are assumed to be spherical with diameters that can be constant or follow a Gaussian distribution.

Table 3.1: Simulation parameters and material properties of SS316L using in the DEM model

Particle's properties	Values	Refs
Density (kg/m^3)	7800	[140]
Young's modulus (GPa)	1.1	–
Poisson's ratio	0.3	[140]
Coefficient of friction	1.0	[103]
Coefficient of restitution	0.3	–

3.1.3. Simulation steps

DEM has been commonly employed to model the powder bed in the SLM process [54, 131]. In this work, the deposition of powder particles was performed in LIGGGHTS[®] [119]. LIGGGHTS[®] is an open-source software package providing a platform to calculate the movements and the heat transfer in particulate materials. The powders were considered as solid spheres with their radii following a Gaussian distribution. Gravitational and contact forces were exerted on each particle, and the motions of particles were calculated based on Newton's second law.

The powder bed was formed by randomly generating a cloud of powders and dropping freely onto the substrate to form a deposited powder bed. A blade was then moved across the powder bed to generate a uniform layer thickness of powder.

3.1.4. Powder bed generation

3.1.4.1. Uniform powder bed

Figure 3.2: Powder bed deposition model with powder size of $27 \pm 10 \mu\text{m}$ viewed from (a) the front at $t = 0$ s, (b) the front at $t = 0.036$ s, (c) the front at $t = 1.12$ s, (d) the front at $t = 1.6$ s and (e) the top at $t = 1.6$ s.

The 3D computational domain had a dimension of $x \times y \times z = 2100 \times 800 \times 600 \mu\text{m}^3$, where the gravitational force is along the y -axis. The cloud of 1800 powder particles was modelled and inserted at the area above $y = 300 \mu\text{m}$. Figures 3.2(a) to (e) illustrate the snapshots of the powder depositing onto the substrate from $t = 0$ to $t = 1.6$ s. Due to the gravitational force, all the particles settled down and reached equilibrium at $t = 0.036$ s. After that, a blade having a size of $x \times y \times z = 10 \times 750 \times 600 \mu\text{m}^3$ was employed such that the top of the blade was located at $y = 800 \mu\text{m}$. A velocity of 0.001 m/s was set to control the blade moving from left to right. Due to the recoating of the blade, a uniform powder layer thickness of 50 μm was formed.

3.1.4.2. Powder bed containing overhanging features

To simulate the powder bed containing an overhanging feature, an additional block of SS316L were modelled and it sits on the substrate. The block acts as already-melted and solidified powder. It also comes in different shapes and sizes – cuboid and 40°-inclined for different investigations as depicted in Figure 3.3. The inclined angle was formed between the down surface and the z -axis. In addition in overhang printing, two common strategies, namely perpendicular printing and parallel printing, exists [141]. Thus, the powder was deposited onto different types of blocks: cuboid block for perpendicular printing (see Figure 3.3(a)), cuboid block for parallel printing (see Figure 3.3(b)), and 40°-inclined block for parallel printing (refer to Figure 3.3(c)). The geometry and dimensions of the blocks are depicted in Figure 3.3. The blocks were generated from SOLIDWORKS® [142]. After that, the STL files were exported to LIGGGHTS® to simulate the powder deposition and recoating of the powder bed on the blocks.

Figure 3.3: Schematic of (a) cuboid block for perpendicular printing, (b) cuboid block for parallel printing, and (c) 40° -inclined block viewed from (i) the tilted-view, and (ii) the side.

Figure 3.4: Powder deposited on (a) cuboid block for perpendicular printing, (b) cuboid block for parallel printing , and (c) 40° -inclined block for parallel printing viewed from (i) the top, and (ii) the front, and (iii) the side at cross-section of $x = 1700\ \mu\text{m}$ at $t = 2.76\ \text{s}$ with powder size of 20 to $53\ \mu\text{m}$.

The dimensions of the model were $x \times y \times z = 3500 \times 1500 \times 600 \mu\text{m}^3$ and the dimensions of deposition platform, blade and blocks can be found in Figure 3.3. Clouds of 13500, 16000 and 16000 powder particles were modelled and inserted in the simulation domain of the deposition on cuboid block for perpendicular printing, cuboid block for parallel printing and 40°-inclined block respectively. The clouds of powder were modelled at $y = 500 \mu\text{m}$ and above. In the overhang simulation, a blade where its bottom is located at $y = 350 \mu\text{m}$ was employed to form a uniform powder layer thickness of $50 \mu\text{m}$ on the blocks. Figure 3.4 depicts the powder beds containing overhanging features where the powder size ranges from 20 to $53 \mu\text{m}$ following the Gaussian distribution. The powder was deposited on cuboid blocks as seen in Figures 3.4(a) and (b). In addition, the deposition of powder bed on the 40°-inclined block is also depicted in Figure 3.4(c).

3.1.4.3. Powder bed with different sizes of powder

The SLM process is available to different materials with different powder sizes classified as fine, medium-fine and coarse as listed in Table 3.2. In the simulation, these classes of powder were deposited on a 40°-inclined block as an example. The model, however, is also able to deposit different classes of powder on a substrate or on cuboid blocks which are not further discussed in this section. The 3D domain of $x \times y \times z = 3500 \times 1500 \times 600 \mu\text{m}^3$ were modelled, where the gravity is along the y-axis. Due to the gravitational force, the powder was dropped freely on the substrate and on the 40°-inclined block. Then a blade moving along the x -axis form a uniform layer thickness of $50 \mu\text{m}$ on the 40°-inclined block as depicted in Figure 3.5.

Figure 3.5: Deposited powder bed on the 40^o-inclined block using (a) fine, (b) medium-fine and (c) coarse powder.

Table 3.2: Classification of SS316L powder used in simulation

Powder classification	Type	Powder distribution	Powder size (μm)	Percent (%)	Ref.
Fine powder	1	uniform	15	50	[70]
	2	Gaussian	15 to 30	40	
	3	Gaussian	30 to 35	10	
Medium-fine powder	4	Gaussian	20 to 53	100	[143]
Coarse powder	5	Gaussian	45 ± 10	100	[35]

3.1.4.4. Multi-layer deposition

In the SLM process, after the first layer was melted and solidified, the second layer of powder will be deposited on top of the first layer. Then, the laser beam will scan the second layer of powder. The process is repeated until the 3D object is formed. In this work, the simulation imitates the deposition of a subsequent layer of powder on top of a first melted layer as seen in Figure 3.6. Firstly, the information of the first melted layer (see Figures 3.6(a) and (b)) is saved in the STL file and exported to LIGGGHTS[®]. This STL file was defined as a second mesh/boundary in the lower y-axis, and the second mesh/boundary was bounded inside the dashed lines as depicted in Figure 3.6. The first mesh/boundary in lower y-axis was representative of the deposition platform. All the particles were dropped freely and allowed to settle down. When the powder settled on the second mesh, it formed the second layer of powder. The rest of the powder would be rested on the first mesh. Figures 3.6(c) to (f) illustrate the deposition of powder at different time-steps. The technique can also be applied to the deposition of the subsequent layers.

Figure 3.6: Morphology of (a) first scanned layer viewed from the top and (b) melt track contour at cross-section of $z = 200 \mu\text{m}$ and the powder deposition of the subsequent layer at cross-section of $z = 200 \mu\text{m}$ at (c) $t = 0.01 \text{ s}$, (d) $t = 0.04 \text{ s}$, (e) $t = 2 \text{ s}$ and (f) $t = 2.68 \text{ s}$. The dashed lines indicates the region where the second layer of powder is deposited.

3.2. CFD model

After the powder bed was deposited by employing the DEM, the powders' radii and coordinates were exported to OpenFOAM® [144] which will then generate the powder particles on the substrate. The CFD simulation on laser interaction, phase-change and melt pool dynamics was then performed.

3.2.1. Heat transfer and melt flow dynamics model

The CFD model was used to simulate laser-powder bed interaction, phase-change, heat and mass transfer, and fluid flow of the melt track. By employing the VOF method, the model was able to capture the interface between the metal and gas. In this study SS316L, which was widely used in SLM, was chosen as the material of the powder and substrate [21]. As such, the existing reported experimental results of SLM of SS316L can be used for validating and comparing to the simulation. The metallic and gaseous phases were determined by α_1 and $(1-\alpha_1)$ respectively. $\alpha_1 = 1$ indicates a cell completely occupied by the metallic phase and $\alpha_1 = 0$ represents a fully gaseous cell. Any value between 0 and 1 means that the material is undergoing melting. A temperature dependent variable γ is employed to represent the solid or liquid state of the metal cells, and is described as [145]

$$\gamma = \begin{cases} 0 & , \quad T \leq T_s \\ \frac{T - T_s}{T_l - T_s} & , \quad T_s < T < T_l \\ 1 & , \quad T \geq T_l \end{cases} \quad (3.19)$$

where T_s and T_l are solidus and liquidus temperature of the metal powder respectively and T is the temperature field of the computational domain. Hence, the volume fraction of solid metal f_s

and liquid metal f_l are $\alpha_1(1-\gamma)$ and $\alpha_1\gamma$ respectively. Consequently, the material properties $\bar{\varphi}$ of each cell are calculated as [81]

$$\bar{\varphi} = \alpha_1(1-\gamma)\varphi_s + \alpha_1\gamma\varphi_l + (1-\alpha_1)\varphi_g, \quad (3.20)$$

where φ_s , φ_l , and φ_g are the material property in solid, liquid and gaseous phase respectively.

The volume fraction of the metallic phase satisfies the following conservation equation

$$\frac{\partial(\bar{\rho}\alpha_1)}{\partial t} + \nabla \cdot (\bar{\rho}\mathbf{u}\alpha_1) = 0, \quad (3.21)$$

where $\mathbf{u}$ is the flow velocity, t is time, and $\bar{\rho}$ is the volume average density.

The mass conservation is calculated as

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho}\mathbf{u}) = 0, \quad (3.22)$$

while the momentum equation is computed as [81, 146]

$$\frac{\partial \bar{\rho}\mathbf{u}}{\partial t} + \nabla \cdot (\bar{\rho}\mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) - K_c \left[\frac{(1-f_l)^2}{f_l^3 + c_k} \right] \mathbf{u} + \bar{\rho}\mathbf{g} + \mathbf{F}_{st} + \mathbf{F}_M + \mathbf{P}_r, \quad (3.23)$$

where p is the pressure, μ is the dynamic viscosity and $\mathbf{g}$ is gravitational acceleration. The

Darcy's term, $-K_c \left[\frac{(1-f_l)^2}{f_l^3 + c_k} \right] \mathbf{u}$, is the damping term in the mushy zone, where K_c and c_k are

permeability coefficient and a small constant respectively. The surface tension force $\mathbf{F}_{st}$ is written as

$$\mathbf{F}_{st} = \sigma \kappa \mathbf{n} |\nabla \alpha_1| \frac{2\bar{\rho}}{\rho_s(1-\gamma) + \rho_l\gamma + \rho_g}, \quad (3.24)$$

where σ , κ , and $\mathbf{n}$ are surface tension coefficient, surface curvature and unit normal respectively. $|\nabla\alpha_1|$ was adopted to transform an interfacial per unit into a volumetric surface

force. The term $\frac{2\bar{\rho}}{\rho_s(1-\gamma)+\rho_l\gamma+\rho_g}$ is used to redistribute the interfacial force towards the

heavier metal phase. The surface tension σ of the metallic material is described as [147]

$$\sigma = \sigma_s^0 - A(T - T_s) - RT\Gamma_s \ln(1 + k_1 a_i e^{-\Delta H^0/RT}), \quad (3.25)$$

where σ_s^0 is the surface tension of pure metal at the melting point (solidus temperature), A is the surface tension gradient for pure metal, R is gas constant, Γ_s is surface excess at saturation, k_1 is entropy factor, a_i is weight percent of sulfur, and ΔH^0 is the heat absorption. The unit normal vector and the curvature of metal/gas interface can be expressed as

$$\mathbf{n} = \frac{\nabla\alpha_1}{|\nabla\alpha_1|}, \text{ and} \quad (3.26)$$

$$\kappa = -\nabla \cdot \mathbf{n}. \quad (3.27)$$

The Marangoni force $\mathbf{F}_M$ is defined as

$$\mathbf{F}_M = \frac{d\sigma}{dT} (\nabla T - \mathbf{n}(\mathbf{n} \cdot \nabla T)) |\nabla\alpha_1| \frac{2\bar{\rho}}{\rho_s(1-\gamma)+\rho_l\gamma+\rho_g}, \quad (3.28)$$

where $\frac{d\sigma}{dT}$ describes the surface tension gradient of SS316L. The recoil pressure $\mathbf{P}_r$ is described

by

$$\mathbf{P}_r = 0.54P_0 \exp\left[\frac{L_v M (T - T_v)}{RTT_v}\right] \mathbf{n} |\nabla\alpha_1| \frac{2\bar{\rho}}{\rho_s(1-\gamma)+\rho_l\gamma+\rho_g}, \quad (3.29)$$

where P_0 is ambient pressure, L_v is the latent of vaporization, T_v is the evaporation temperature, and M is the molar mass.

The last three forces on the right hand side of Eq. (3.23) are the surface tension force, $\mathbf{F}_{st}$, Marangoni force, $\mathbf{F}_M$, and the recoil pressure, $\mathbf{P}_r$. The surface tension force, $\mathbf{F}_{st}$, plays a role in minimize the surface area of the liquid metal. For example, when the laser scans the melt track, it forms a recess or keyhole. At the same time, the surface tension force pulls the molten metal to the keyhole to fill up the keyhole. However, the surface tension force is not strong enough to fully fill up the keyhole, thus a recess is always remained at the end of the melt track. Next, Marangoni force, $\mathbf{F}_M$, is calculated based on the surface tension gradient of materials which can be positive or negative. When the material has negative surface tension gradient like SS316L, the Marangoni force will deliver the molten metal from the hot melt pool to the cold tail. On the other hand, the Marangoni force will pull the molten metal from the edge to the centre of the melt pool when the material has the positive surface tension coefficient. Regarding to recoil pressure $\mathbf{P}_r$, it becomes active when the temperature of the metal/gas interface reach the boiling point. Once it happens, the recoil pressure will strongly penetrate the molten metal to form a deep keyhole. During the SLM process, these three forces have major impact on the melt track geometry and the melt pool dynamics.

The energy conservation is expressed as [66, 131]

$$\frac{\partial \bar{\rho} h}{\partial t} + \nabla \cdot (\bar{\rho} \mathbf{u} h) = \nabla \cdot (D_f \nabla h) + q_{abs} - q_{loss} |\nabla \alpha_1| \frac{2\bar{\rho}}{\rho_s(1-\gamma) + \rho_l\gamma + \rho_g}, \quad (3.30)$$

where h is the specific enthalpy, q_{abs} is the absorbed heat from the laser beam. The diffusion coefficient, D_f , is given as

$$D_f = (1 - \alpha_l) \frac{k_g}{C_p} + \alpha_l \frac{k_s \alpha_l (1 - \gamma_l) + k_l \alpha_l \gamma}{C_p}, \quad (3.31)$$

where k and C_p are thermal conductivity and specific heat, respectively. The heat loss at the metal/gas interface is described by $q_{loss} = q_{conv} + q_{rad} + q_{evap}$ [148]. The convection heat loss is computed as $q_{conv} = h_c(T - T_\infty)$, where h_c is convection coefficient and T_∞ is ambient temperature. $q_{rad} = \varepsilon \sigma_B (T^4 - T_\infty^4)$ is the radiation heat loss, where ε is emissivity and σ_B is the Stefan-Boltzmann constant. The evaporation heat loss is calculated as

$$q_{evap} = \frac{0.82 L_v}{\sqrt{2\pi M R T}} P_0 \exp\left[\frac{L_v (T - T_v)}{R T T_v}\right], \text{ where } M \text{ is the molar mass [149].}$$

In this model, the heat capacity C_p is described as [58]

$$C_p = \begin{cases} C_{ps0} + C_{psCoeff} T & , \quad T \leq T_s \\ \frac{h_s}{T_l - T_s} & , \quad T_s < T < T_l \\ C_{pl} & , \quad T \geq T_l \end{cases} \quad (3.32)$$

where $C_{ps} = C_{ps0} + C_{psCoeff} T$ is the temperature-dependent heat capacity of the solid phase, and h_s is the latent heat of fusion. Furthermore, the temperature T is calculated based on the enthalpy h . When the temperature is lower than the solidus temperature, the enthalpy h is calculated as

$$h(T) - h(T_{ref}) = \int_{T_{ref}}^T C_p dT, \quad (3.33)$$

where T_{ref} is the reference temperature which was set as 300 K. Thus, the relationship between the enthalpy h and the temperature T is described as [150]

$$T = \begin{cases} \frac{-C_{ps0} + \sqrt{C_{ps0}^2 + 2C_{psCoeff}(C_{ps0}T_{ref} + 0.5C_{psCoeff}T_{ref}^2 + h)}}{C_{psCoeff}}, & h \leq h(T_s) \\ T_s + \frac{h - h(T_s)}{h_s}(T_l - T_s), & h(T_s) < h \leq h(T_s) + h_s \\ T_l + \frac{(h - h(T_s) - h_s)}{C_{pl}}, & h > h(T_s) + h_s \end{cases} \quad (3.34)$$

where $h(T_s) = C_{ps0}(T_s - T_{ref}) + 0.5C_{psCoeff}(T_s^2 - T_{ref}^2)$.

Hence, by calculating Eqns. (3.30-3.34), the temperature field is computed.

3.2.2. Material properties

The material used in this work is SS316L and its thermo-physical properties can be determined by $\Phi = a + bT + cT^2$ [58, 151], where Φ is the material property, T is temperature, and a , b , and c are constant coefficients. Table 3.3 lists the material properties of SS316L used in the CFD simulation model.

Table 3.3: Material properties of SS316L and coefficients applied in the simulation

Material property	Symbol	Value	Ref.
Density of solid metal (kg/m ³)	ρ_s	7900	[62]
Density of liquid metal (kg/m ³)	ρ_l	$7433 + 0.0393T - 1.8 \times 10^{-4}T^2$	[58]
Specific heat of solid metal (Jkg ⁻¹ K ⁻¹)	C_{ps}	$462 + 0.134T$	[58]
Specific heat of liquid metal (Jkg ⁻¹ K ⁻¹)	C_{pl}	775	[58]

Thermal conductivity of solid metal ($\text{Wm}^{-1}\text{K}^{-1}$)	k_s	$9.248+0.01571T$	[58]
Thermal conductivity of liquid metal ($\text{Wm}^{-1}\text{K}^{-1}$)	k_l	$12.41+0.003279T$	[58]
Thermal conductivity of air ($\text{Wm}^{-1}\text{K}^{-1}$)	k_g	0.03	[152]
Boiling temperature (K)	T_v	3090	[148]
Solidus temperature (K)	T_s	1658	[148]
Liquidus temperature (K)	T_l	1723	[148]
Molar mass (kgmol^{-1})	M	0.05593	[148]
Viscosity of liquid metal ($\text{kgm}^{-1}\text{s}^{-1}$)	μ	6×10^{-3}	[62]
Permeability coefficient ($\text{kgm}^{-3}\text{s}^{-1}$)	K_c	1×10^{12}	
Surface tension of pure metal at melting point (Nm^{-1})	σ_s^0	1.943	[147]
Temperature coefficient of surface tension ($\text{Nm}^{-1}\text{K}^{-1}$)	A	4.3×10^{-4}	[147]
Surface excess at saturation	Γ_s	1.3×10^{-8}	[147]
Entropy factor	k_1	0.00318	[147]
Weight percent of sulfur (%)	a_i	0.00	—
Heat of fusion (m^2s^{-2})	h_s	2.7×10^5	[153]
Latent heat of vaporization (m^2s^{-2})	L_v	7.45×10^6	[148]
Atmosphere pressure (Nm^{-2})	P_0	101,000	[148]

Universal gas constant ($\text{kgm}^2\text{s}^{-2}\text{K}^{-1}\text{mol}^{-1}$)	R	8.314	[148]
Stefan-Boltzmann's constant ($\text{Wm}^{-2}\text{K}^{-4}$)	σ_B	5.67×10^{-8}	[148]
Emissivity	ε	0.4	[63]
Convection coefficient ($\text{kgs}^{-3}\text{K}^{-1}$)	h_c	80	[148]
Power distribution factor	f	2	[154]
Beam radius (μm)	r	40	[154]
Absorption coefficient	η	0.32	[58]
Reflective index of SS316L at wavelength of 1 μm	n	$3.27+i4.48$	[155]

3.2.3. Coupling of CFD-DEM model

Currently, the DEM solver and the CFD solver are coupled manually. Firstly, the deposition of the powder is simulated in the DEM model. Then, the information of powder' radii and coordinates are exported to the CFD model. In the CFD model, the powder particles are considered as stationary particles during the melting and solidification of the melt track. Once the melt track is fully solidified, the top surface of the melt track is saved in the STL file to transfer geometry of the melted layer to the DEM model for the next layer simulation. In fact, the powder/powder, powder/air and powder/melt pool interactions during the melting and solidification process have not been considered. It will be further studied in the future works.

3.3. Laser heat source model

To improve the accuracy of the computational model in SLM, the laser heat source is required to simulate precisely. In fact, most simulation works assumed only the top surface of the powders covered by the laser beam spot is heated [54, 146]. This simplified heat source model calculated the laser power intensity, which was then applied on the top surface of the powder bed. This model is suitable to simulate conduction-mode, transient-mode, and medium-deep keyhole-mode melt pool. Furthermore, most of the simulation works assumed a constant absorption coefficient of the laser heat source [54, 59, 63]. However, as reported by Trapp *et al.*, the absorption coefficient is a function of the laser power and scanning speed [156]. Therefore, the assumption of constant absorption coefficient becomes inadequate at some regions, especially when the melt track is in the well-deep keyhole-mode. Furthermore in reality, multiple reflections of the laser in the keyhole determine how the energy is actually transferred. Therefore, the simplified heat source model may be inadequate in certain situations. As a result, the ray-tracing model was developed to simulate the keyhole-mode melt pool with high accuracy. Unfortunately, to model a same domain size, the ray-tracing model takes longer time. Thus, based on the applications, simplified heat source model and ray-tracing model can be used alternately.

3.3.1. Simplified heat source model

3.3.1.1 Gas/metal interface cell identification

In the model, an absorption index f_{absorb} is employed to identify the top gas/metal interface cells. The program searches for the top gas/metal interface cells from top to the bottom along the y-axis. A variable $f_{indicator}$ is adopted to compare and define f_{absorb} . Initially, $f_{indicator}$ is set as 1 and f_{absorb} is set as 0. Cells with α_1 greater than 0.05 will be identified as gas/metal interface cell. A

condition loop based on $f_{indicator}$, α_1 and f_{absorb} was used. When a cell is in gaseous phase, $f_{indicator}$ and f_{absorb} remain unchanged as the initial setup. However, when the cell is identified to be along the gas/metal interface, the value of f_{absorb} and $f_{indicator}$ will be updated with $f_{absorb} = \alpha_1$ and $f_{indicator} = f_{indicator} - \alpha_1$. Then, the loop continues for the next cell along the y-axis. As long as $f_{indicator} \geq \alpha_1$, then f_{absorb} and $f_{indicator}$ was set as $f_{absorb} = \alpha_1$ and $f_{indicator} = f_{indicator} - \alpha_1$. However, if $f_{indicator} < \alpha_1$, then $f_{absorb} = f_{indicator}$ and $f_{indicator} = 0$.

3.3.1.2. Simplified heat source of the laser beam

The laser beam center was initially located at $c_{beam,0} = (x_0, z_0)$ and the laser beam plane was set parallel to the substrate plane as depicted in Figure 3.7. The laser beam intensity profile assumes a Gaussian distribution with the beam power density expressed as

$$I = \frac{2\eta P_{laser}}{\pi r^2} \exp\left(\frac{-2w^2}{r^2}\right), \quad (3.35)$$

where P_{laser} is the laser power, r is the beam spot radius, w is the distance from the calculation cell to the beam centre and η is the absorptivity coefficient [62]. Therefore, the heat input from the laser beam to the top gas/metal interface cells is approximated as

$$q_{laser} = \frac{f_{absorb} I}{\Delta y}, \quad (3.36)$$

where Δy indicates the size of the numerical grid. By employing the laser beam with the beam radius of $40 \mu\text{m}$ and the mesh grid sizes of $4 \times 4 \times 4 \mu\text{m}^3$, the simplified heat source model is able to simulate 98.1% of the total laser power.

Figure 3.7: A schematic diagram of the laser beam in the simulation model

3.3.2. Ray-tracing model

Ray-tracing model is employed to simulate the reflection of laser rays. Physically, one laser beam contains countless of laser rays. When the incident ray touches the gas/metal interface, it will reflect in different direction depending on the angle between the normal vector of the gas/metal interface and the incident ray. The model keeps tracking the path of the laser rays until its power can be neglectable or the laser rays go outside of the domain. The laser heat source model plays the role of imitating the movement of a laser beam with the power of P_{laser} and the beam radius of r . The laser moves at a velocity of v_0 , with the laser beam center at coordinates $c_{beam,0} = (x_0, z_0)$ as depicted in Figure 3.7. The laser beam was assumed as a Gaussian heat source with the distribution factor f of two. The ray-tracing algorithm firstly identified all the metallic cells at the gas/metal interface cells. The initial laser rays were subsequently generated according to the laser beam profile. Finally, the ray-tracing procedure was performed to track the travelling and reflection of laser rays. The details are described in the following sections.

3.3.2.1. Gas/metal interface cell identification

In the model, the gas/metal interface cells are identified by using the volume fraction of the metallic phase α_1 , and Figure 3.8 illustrates the gas/metal interface cells of the powder bed.

Figure 3.8: Schematic of gas/metal interface cells

The cell is considered as a gas/metal interface cell when it satisfies the following conditions

$$\begin{cases} \alpha_1 \geq 0.5 \\ |\nabla \alpha_1| > \varepsilon / \Delta x = 0.05 / \Delta x \end{cases}, \quad (3.37)$$

where Δx is the cell width or so-called grid size, and ε is a small arbitrary number (0.05). Firstly, only those cells containing metal phases ($\alpha_1 \geq 0.5$) may absorb the power during the laser scanning process. Secondly, as for the VOF method, the gradient of α_1 is inversely proportional

to the grid size and is only non-zero at the interface. In this work, the gradient of α_1 can be evaluated by

$$\nabla \alpha_1 = \left(\frac{\partial \alpha_1}{\partial x}, \frac{\partial \alpha_1}{\partial y}, \frac{\partial \alpha_1}{\partial z} \right), \quad (3.38)$$

where $\frac{\partial \alpha_1}{\partial x} \Big|_{i,j,k} = \frac{\alpha_1|_{i+1,j,k} - \alpha_1|_{i-1,j,k}}{2\Delta x}$, $\frac{\partial \alpha_1}{\partial y} \Big|_{i,j,k} = \frac{\alpha_1|_{i,j+1,k} - \alpha_1|_{i,j-1,k}}{2\Delta y}$, and

$$\frac{\partial \alpha_1}{\partial z} \Big|_{i,j,k} = \frac{\alpha_1|_{i,j,k+1} - \alpha_1|_{i,j,k-1}}{2\Delta z}.$$

Around the interface, α_1 typically changes from 0 to 1 within two or three cells. Therefore, the second condition can be used to find the interface.

3.3.2.2. Rays generation

The laser beam output from the laser fiber optical connector is a collimated beam. After passing through the 3-axis laser scanning system which includes a dynamic focusing system and a two-mirror beam directing system, the laser beam becomes a focused beam. However, due to the large working distance (distance between the laser scanning system and the powder bed layer), the beam profile can be approximated/assumed to be collimated in the simulations.

Figure 3.9: Schematic diagram of (a) the beam calculating area and (b) sub-rays at the center of the laser beam.

The laser beam center was initially located at $c_{beam,0} = (x_0, z_0)$ and the laser beam plane was set parallel to the substrate plane. Starting from the center of the laser beam, the algorithm firstly searched for the cells within $1.6r$ of the beam as depicted in Figure 3.9(a) in order to capture 99.44% of the total laser power. The rays from the laser were then generated for each cell. Each

ray contains the information of ray center A_j^i , ray direction $\mathbf{u}_j^i$, times of reflection i^{th} , and laser ray power P_j^i , where j indicates ordinal ray number, and i represents the number of times the laser ray is reflected, where $i = 0$ represents an incident laser ray without reflection. For SS316L with the reflective index of $n = 3.24 + 4.28i$, the absorption coefficient is around 0.3 [58]. After a laser ray undergoes 13 times of reflections, the remaining power becomes negligible (around 1%) as compared to the initial ray power. Therefore in this work, the ray-tracing procedure for a laser ray terminates when the number of reflections reaches 13. Initially, all rays were given an initial direction of $\mathbf{u}_j^0 = (0, -1, 0)$. Moreover, the initial power P_j^0 of each ray is given by

$$P_j^0 = \frac{fP_{laser}}{\pi r^2} \exp \left[-f \frac{(x_{cj} - v_0 t - x_0)^2 + (z_{cj} - z_0)^2}{r^2} \right] \Delta x^2. \quad (3.39)$$

3.3.2.3. The interaction between the ray and the cells

A single laser ray is employed to explain the absorption and reflection of the laser ray as shown in Figure 3.10. The laser ray has the starting point of $A_j^i = (x_j^i, y_j^i, z_j^i)$ with the unit vector of laser ray direction of $\mathbf{u}_j^i = (ux_j^i, uy_j^i, uz_j^i)$ as shown in Figure 3.10(a). The vector from the center of the gas/metal interface cell k , which is denoted by $B_k = (x_{B,k}, y_{B,k}, z_{B,k})$, to the starting of ray j is therefore calculated as

$$\mathbf{d}_{2k,j} = (x_{B,k} - x_j^i, y_{B,k} - y_j^i, z_{B,k} - z_j^i). \quad (3.40)$$

The unit vector from A_j^i to B_k is defined as

$$\mathbf{u}_{k,j}^i = \frac{\mathbf{d}_{2k,j}}{|\mathbf{d}_{2k,j}|}. \quad (3.41)$$

Figure 3.10: Schematic of (a) gas/metal interface cells, (b) gas/metal interface cells along the laser beam, (c) incident cell and the neighbor cells and (d) reflected laser beam.

The angle θ_j^i between the vector $\mathbf{u}_j^i$ and $\mathbf{u}_{k,j}^i$ is expressed as

$$\theta_j^i = \arccos \left(\frac{\mathbf{u}_j^i \mathbf{u}_{k,j}^i}{|\mathbf{u}_j^i| |\mathbf{u}_{k,j}^i|} \right). \quad (3.42)$$

Therefore, the perpendicular distance from B_k to ray j is given as

$$d_{1k,j}^i = |\mathbf{d}_{2k,j}^i| \sin(\theta_j^i). \quad (3.43)$$

Then, the program searches for the gas/metal interface cells along the ray path. Cell k is considered as gas/metal interface cell along the ray path when the distance $d_{1k,j}^i \leq \sqrt{3}/2 \Delta x$ as depicted in Figure 3.10(b). Among the gas/metal interface cells along the ray path, the cell with the shortest $|\mathbf{d}_{2k,j}^i|$ is chosen as corresponding interface cell where the laser heat source is mainly absorbed as illustrated in Figure 3.10(c). Subsequently, the program calculates the Fresnel absorption coefficient which is computed as [157]

$$\eta = 1 - \frac{1}{2} \left[\frac{(\text{Re}_{ref} \cos \psi_j^i - 1)^2 + (\text{Im}_{ref} \cos \psi_j^i)^2}{(\text{Re}_{ref} \cos \psi_j^i + 1)^2 + (\text{Im}_{ref} \cos \psi_j^i)^2} + \frac{(\text{Re}_{ref} - \cos \psi_j^i)^2 + \text{Im}_{ref} \text{Im}_{ref}}{(\text{Re}_{ref} + \cos \psi_j^i)^2 + \text{Im}_{ref} \text{Im}_{ref}} \right], \quad (3.44)$$

where Re_{ref} and Im_{ref} are the reflective index n of the material. The symbol ψ_j^i is the angle between the incident laser ray and the surface normal vector $\mathbf{n}_k$ of cell k , and it is described as [158]

$$\psi_j^i = \arccos(-\mathbf{u}_j^i \mathbf{n}_k). \quad (3.45)$$

As a result, the corresponding interface cell at which the laser ray directly irradiates and its neighbouring cells will absorb the laser power of $P_{j,k,abs}^i = \eta P_j^i$ (see Figure 3.10(c)) based on the distribution index given as [158]

$$w_k = \begin{cases} 1 & , \quad k \equiv (m, n, p) \\ 0.3 & , \quad k \equiv (m \pm 1, n, p), (m, n \pm 1, p), (m, n, p \pm 1) \end{cases} \quad (3.46)$$

where (m, n, p) denotes the corresponding interface cell, and the neighboring cells are $(m \pm 1, n, p)$, $(m, n \pm 1, p)$ and $(m, n, p \pm 1)$ as depicted in Figure 3.11.

Figure 3.11: Schematic of corresponding interface cell and neighbor cells

The heat source from ray j is applied to each cell and is calculated as

$$q_{j,k,abs} = \frac{\eta P_j^i \alpha_{1,k}}{\alpha_1(m, n, p) + 0.3\alpha_1(m \pm 1, n, p) + 0.3\alpha_1(m, n \pm 1, p) + 0.3\alpha_1(m, n, p \pm 1)}, \quad (3.47)$$

if the cell is the corresponding interface cell. However, if the cell is a neighboring cell, the heat source is then computed as

$$q_{j,k,abs} = \frac{0.3\eta P_j^i \alpha_{1,k}}{\alpha_1(m, n, p) + 0.3\alpha_1(m \pm 1, n, p) + 0.3\alpha_1(m, n \pm 1, p) + 0.3\alpha_1(m, n, p \pm 1)}. \quad (3.48)$$

Hence, the total heat absorbed into cell k is $q_{k,abs} = \sum_{j=1}^{\max j} q_{j,k,abs}$. This value is then used in Eqns.

(3.30) and (3.34) to calculate the temperature field.

Then, the information of the laser ray j at the reflected time $(i+1)^{th}$ is updated, with the laser power of $P_j^{i+1} = (1-\eta)P_j^i$, and the starting point $A_j^{i+1} \equiv B_k$ as seen in Figure 3.10(d). In addition, the direction of the laser ray j at the reflection $(i+1)^{th}$ is calculated as [49]

$$\mathbf{u}_j^{i+1} = \mathbf{u}_j^i - 2(\mathbf{u}_j^i \cdot \mathbf{n}_k)\mathbf{n}_k, \text{ and } \mathbf{u}_j^{i+1} = \frac{\mathbf{u}_j^{i+1}}{|\mathbf{u}_j^{i+1}|} \quad (3.49)$$

The reflection process will continue until the laser ray power is close to zero or the number of reflections is greater than 13.

3.4. Validation of CFD model using simplified heat source of the laser beam

3.4.1. Validation setup

The 3D computational domain had a dimension of $x \times y \times z = 1000 \times 300 \times 240 \mu\text{m}^3$, where the gravitational force is along the y -axis. The domain consisted of a 200 μm -tall substrate and a 100 μm -tall air layer above the powder bed. The model contains 2,160,000 elements with a constant mesh grid size of $4 \times 4 \times 4 \mu\text{m}^3$. The initial temperature of the domain was set as 300 K.

The single-melt track is printed on a SS316L substrate without powder with the laser powers and scanning speeds are listed in Table 3.4. To simplify the number of variables of the model, the model is validated by using the single-melt track without powder on the substrate. This test is an initial validation work to assure the accuracy of the model.

In the experiment, the samples were printed in SLM[®] 280 HL equipped with two 400W Yb fiber continuous wave (CW) lasers with the wavelength of 1070 nm (see lines 1602 and 2050). As for the experiment part of this work, we only activated one of the two 400W laser to print our samples. During the printing process, the oxygen content inside the chamber was set as 0.2 % controlled by the argon gas. The SS316L substrate with the size of $80 \times 80 \times 8 \text{ mm}^3$ was used to print the single-melt tracks. On top of the substrate, no powder was deposited similar to the simulation model. The 1070 nm Yb fiber laser was focused to a nearly Gaussian beam with a diameter of 80 μm . The melt track with a length of 3 cm was printed on top of the substrate.

Table 3.4: The printing parameters of single-melt track samples

Sample's name	Power (W)	Speed (mm/s)	Power: Speed ratio
S1	200	1600	0.125
S2	100	400	0.25
S3	200	800	0.25
S4	300	1200	0.25
S5	400	1600	0.25
S6	300	1000	0.33
S7	400	1000	0.40

S8

200

400

0.50

3.4.2. Results

In this work, the melt pool depths and widths were used to determine the accuracy of the model. The melt pool depths and widths were measured at three cross-sections at $x = 1100, 1200$ and $1300 \mu\text{m}$. The melt pool depths were measured from the top surface of the substrate and the melt pool widths were taken where its width is largest at the top surface of the substrate. The average values of the melt pool depths and widths at three cross-sections were extracted and compared with the experimental values.

In the experiment, the substrate with the single-melt track was cut at three cross-sections using cutting machine Struers Discotom-10, and mounted for cross-section analysis. Metallographic grinding was performed with sand paper (320 CW, 600 CW, and 1000 CW) followed by automatic polishing using Struers Tegramin-25 with diamond suspension ($9 \mu\text{m}$ and $3 \mu\text{m}$), and finally, silica suspension ($0.04 \mu\text{m}$) was used for final precision polishing. In order to observe the melt pool geometry, etching is required, where a Kroll's reagent etchant was applied. The microscope named Axioskop 2 was employed to visualize the melt pool geometry of the single-melt track. In the experiment, the melt track was cut and measured at three cross-sections. The average melt pool depths and the average melt pool widths were taken and compared to the ones in the simulation.

Table 3.5: The melt pool depths and widths of simulation and experiment of the single-melt tracks

	Depth			Width		
	Simulation	Experiment	Deviation, ε	Simulation	Experiment	Deviation, ε
	(μm)	(μm)	(%)	(μm)	(μm)	(%)
S1	40 ± 2	42.42 ± 5	5.70	104 ± 0	98.76 ± 7	5.31
S2	60 ± 0	51.51 ± 4	16.48	114 ± 2	111.84 ± 10	1.93
S3	80 ± 0	83.04 ± 5	3.66	118 ± 2	120.40 ± 5	1.99
S4	88 ± 0	91.13 ± 4	3.43	134 ± 6	122.27 ± 7	9.59
S5	90 ± 2	95.29 ± 7	5.55	132 ± 4	125.11 ± 12	5.51
S6	102 ± 2	115.84 ± 6	11.95	126 ± 2	123.46 ± 8	2.06
S7	140 ± 0	157.71 ± 8	11.23	138 ± 2	136.69 ± 11	0.96
S8	132 ± 4	212.25 ± 11	37.81	140 ± 4	179.68 ± 9	22.08

From the data shown in Table 3.5, the deviations between the simulated melt pool depths and widths and the experiments are in most cases smaller than 15%, except for sample S8. Furthermore, Figure 3.12 depicts the melt pool geometry of different samples where samples S2, S3, S4 and S5 have the same energy density (see Figures 3.12 (a) to (d)). As noticed, the melt

pools in the simulation and the ones in the experiment share the geometrical similarity. However, sample S8 exhibits high deviations between the simulated melt pool depths and widths and the experiments as listed in Table 3.5. In addition, Figure 3.12(e) shows that melt pool depth in the experiment is much deeper as compared to the one in the simulation. Therefore, it is challenging to achieve deep-keyhole melt pool by employing the simplified heat source model due to the omission of multiple reflections of the laser rays. In order to simulate deep keyhole, it is necessary to simulate the multiple reflections of laser rays. Briefly, the simplified heat source model is suitable for simulating the conduction-mode, transient-mode, and medium-deep keyhole mode.

Figure 3.12: Melt pool geometry of sample (a) S2, (b) S3, (c) S4, (d) S5, and (e) S8 from the (i) simulation at the cross-section of $x = 1050 \mu\text{m}$ and (ii) experiment.

3.5. Validation of CFD model that uses the ray-tracing model

3.5.1. Simulation setup

The consistency between simulations and experiments in the keyhole-mode melting in the SLM process has been examined. The experimental work by Bertoli *et al.* was chosen for comparison [154]. The experiment used gas-atomized Micro-Melt® SS316L powder ranging from 16 to 45 μm in diameter. A near-Gaussian laser beam with a diameter of 55 μm was employed and the layer thickness of the powder bed was kept consistent at 75 μm .

Simulations of single-track melting were performed to model the experiment accordingly. The simulations were carried out with different laser powers and laser scanning speeds as listed in Table 3.6. The 3D simulation domain had a dimension of $x \times y \times z = 1920 \times 600 \times 400 \mu\text{m}^3$, with the direction of the gravity along the y-axis. The simulation domain comprised a 400 μm -tall substrate, 75 μm -thick layer of the powder bed, and a 125 μm -tall layer of air above the powder bed. The powder was assumed to be spherical in shape and follows the Gaussian distribution with the powder diameter ranging from 16 to 45 μm . Each cell size was $4 \times 4 \times 4 \mu\text{m}^3$ in the model. The initial temperature of the domain was set at 300 K. In addition, the laser beam radius was set as 27.5 μm , which follows a Gaussian distribution with the distribution factor of two.

Table 3.6: Laser powers and scanning speeds used in the simulations of single-track melting

Sample	Laser power (W)	Scanning speed (mm/s)	Energy density (J/mm ³)
A	300	1500	48
B	400	2000	48
C	300	900	81
D	500	1500	81
E	300	750	97
F	300	600	121
G	400	800	121
H	200	300	162
K	300	450	162

3.5.2. Results

In this work, the melt pool depths and widths were used to determine the accuracy of the model. The melt pool depths and widths were measured at different cross-sections at $x = 1100, 1200$, and $1300 \mu\text{m}$. The melt pool depths were measured from the top surface of the substrate, and the melt pool widths were taken where its width is largest at the top surface of the substrate. The average values of the melt pool depths and widths of three cross-sections were extracted and compared with the experimental values from the work by Bertoli *et al.* [154] as listed in Table 3.7

Table 3.7: The comparison of the melt pool depth and width in the simulation and the experiment [154]

Sample	Depth			Width		
	Simulation	Experiment	Deviation,	Simulation	Experiment	Deviation,
	(μm)	[154] (μm)	ε (%)	(μm)	[154] (μm)	ε (%)
A	60 ± 0	50	20.00	86 ± 2	85 ± 11	1.18
B	57.3 ± 2.7	64	10.47	92 ± 4	105 ± 18	12.38
C	120 ± 0	128	6.25	100 ± 8	109 ± 21	8.26
D	112 ± 0	123	8.94	100 ± 4	99 ± 33	1.01
E	152 ± 0	146	4.12	112 ± 4	115 ± 25	2.61
F	198 ± 0	198	0.00	114 ± 2	130 ± 29	12.31
G	194 ± 2	220	11.82	108 ± 4	120 ± 22	10.00
H	276 ± 4	266	3.76	110 ± 2	130 ± 10	15.38
K	278 ± 6	302	7.95	110 ± 2	140 ± 25	21.43

Figure 3.13: Melt pool geometry of sample (a) A, (b) C, (c) E, (d) F, and (e) K at cross-section of $x = 1000 \mu\text{m}$.

From the data shown in Table 3.7, the deviations between the simulated melt pool depths and widths and the experiments are in most cases smaller than 15%. Two cases, however, exhibit deviations larger than 15% such as the depth of sample A and width of the sample K. One possible reason could be due to the constant reflective index used in the model, while in reality is dependent on the temperature of the material [159]. In addition, some other constant values like the specific heat of liquid metal is applied constantly at $775 \text{ Jkg}^{-1}\text{K}^{-1}$. However, it should be temperature dependent material properties. As a result, the model is unable to produce the melt pool width as closely to the experiment when the laser penetrates intensively into the substrate.

Furthermore, the effect of energy density on melt pool depth was also simulated as shown in Figure 3.13 which depicts the melt pool geometry of the samples with the same laser power of 300 W at different energy densities of 48, 81, 97, 121, and 162 J/mm^3 . At low energy density of 48 J/mm^3 (see sample A of Figure 3.13(a)), the melt pool is shallow with a depth of $60 \mu\text{m}$. The melt pool depth, however, increases with higher energy density. For example, when the energy

density increases from 81 J/mm^3 (see Figure 3.13(b)) to 162 J/mm^3 (see Figure 3.13(e)), the melt pool depth also increases from $128 \text{ }\mu\text{m}$ to $278 \text{ }\mu\text{m}$.

Separately, a similar trend is observed when the laser power is increased to 400 W which produces deeper melt pool when higher energy density is applied (see Table 3.7). The melt pool depth of sample B with the energy density of 48 J/mm^3 is $57.3 \text{ }\mu\text{m}$, while the melt pool depth of the sample G with the energy density of 121 J/mm^3 is $192 \text{ }\mu\text{m}$. Therefore, the energy density greatly affects the depth of the melt pool, which is consistent with the experiment [154].

3.6. Conclusions

In this work, the DEM model was employed to perform various powder beds to imitate the free surface of the powder bed in the SLM process. The powder could be deposited uniformly on a flat substrate, or it could be deposited on a block such as cuboid block or inclined block. In addition, the powder can be deposited on a previous printed layer to model the subsequent layers. Moreover, different size classes of powder: fine, medium-fine and coarse were modelled.

Additionally, the CFD model was adopted to simulate the complex physics of heat and mass transfer, phase-change, fluid dynamics and laser-powder bed interaction during the SLM process. Two different ways to represent the laser beam – simplified heat source model and ray-tracing model, were employed. The key difference between the simplified heat source model and the ray-tracing model is that in the simplified heat source model, the heat is only applied at the top surface of metal/gas interface. In contrast, the reflection of the laser rays is taken into account on the ray-tracing model. Both models were validated by comparing the melt pool depth and width

of the single melt-track in the simulation to the one in the experiment. It was found that the simplified heat source model is able to achieve high accuracy in simulating the melt pool in the conduction-mode, transient-mode and medium-deep keyhole-mode. However, in order to simulate the melting process happened on top of a thick powder bed or in the well-deep keyhole-mode, the ray-tracing model should be adopted to offer better results in melt pool geometry.

CHAPTER 4: INFLUENCE OF SCANNING STRATEGIES ON THE LEVELNESS OF THE MELT TRACK IN SELECTIVE LASER MELTING PROCESS OF STAINLESS STEEL POWDER USING SIMPLIFIED HEAT SOURCE MODEL

In this chapter, a model using the simplified heat source of the laser beam was employed to study the levelness of multi-track with different scanning strategies. Two common scanning patterns were tested: sequential and boustrophedon. The study found that the sequential scanning strategy leads to a non-flat printed surface, while the boustrophedon strategy produces a flat printed surface. At the beginning of the tracks, molten material was pushed from the keyhole to the rear by the Marangoni force and recoil pressure leading to an increase in the melt pool height of the sequential strategy. On the other hand, due to the high cooling rate when the laser was switched off, a recess was formed at the end of the tracks. Similar phenomenon can be observed in the boustrophedon scanning strategy at the start and end of the track.

4.1. Introduction

In the SLM process, among many processing parameters such as laser power, scanning speed, and layer thickness, scanning strategy plays an important role in affecting the quality of the printed part. Parry *et al.* investigated the influence of the scanning strategies on the generation of the residual stress [96]. The study found that the residual stress is prevalent along the scanning vectors. The influence of scanning strategy on density and metallurgical properties has been studied by Rashid *et al.* [160]. Two scanning strategies namely double scanning strategies and single scanning strategies was employed. The study found the density and the hardness of the

samples can be improved by applying the double scanning strategy. In addition, Ali *et al.* employed both experiment and simulation to study the effect of scanning strategy including scanning vector lengths and scanning vector rotation to on the residual stress of the Ti6Al4V part printed by the SLM process [90]. The study found that the lowest residual stress is generated in the part printed by adopting 90° alternating scanning strategy where the orientation of each layer is turning by 90° comparing to the previous layer. Apart from the above, Thijs *et al.* conducted an experimental study on the scanning strategy effects on the microstructure, texture and the porosity in the parts [73]. The study found that irregular pores can easily be observed at the end of the scan track.

Additionally, computational models have been employed to further understand the SLM process. Chen *et al.* employed a FEM model to investigate the temperature distributions and the melt pool profiles under different scanning strategies, namely unidirectional scanning and alternate scanning [161]. The study found that the melt pool becomes larger from the first scan line to the last. In addition at the U-turn area scanned by the alternate strategy, the previous scanned line have not fully solidified, and it can merge together with the current melt pool. Therefore, a larger melt pool is formed. Moreover by applying the FEM model, Li *et al.* studied the distortion under different scanning strategies [162]. The study found that horizontal pattern produces a smallest distortion along the longitudinal direction. On a contrary, the vertical pattern gives rise to the deflection along the longitudinal axis. Furthermore, the chessboard scanning pattern is preferred to reduce the part distortion.

As discussed, the formation of multi-track has been examined by both simulation and experiment [54, 131]. However, the influence of the scanning strategies on the melt pool dynamics has not been adequately investigated. In this work, an attempt is made to study the influence of the scanning strategies on the melt pool dynamics by using CFD to mimic the melting and solidification process of 316L stainless steel powder during SLM. The aims of this work are to observe the levelness of printed surface based on different scanning strategies.

4.2. Simulation setup

The 3D computational domain had a dimension of $x \times y \times z = 1000 \times 300 \times 600 \mu\text{m}^3$ as described in Figure 4.1, where the gravitational force is along the y -axis. The domain consisted of a 200 μm -tall substrate, a 50 μm -tall powder layer, and a 50 μm -tall air layer above the powder bed. The powder bed distribution was imported from the DEM model. The details of the powder bed generation can be found in section 3.1.4.1. The CFD model contains 2,812,500 elements with a constant mesh grid size of $4 \times 4 \times 4 \mu\text{m}^3$. The initial temperature of the domain was set as 300 K. In the CFD model, the laser beam was modelled as a simplified heat source applied in the top surface of the powder bed. The details of the simplified heat source model can be found in section 3.3.1.

Figure 4.1: Simulation domain with $x \times y \times z = 1000 \times 300 \times 600 \mu\text{m}^3$. The model comprises 200 μm thickness of substrate, 50 μm thickness of powder, and a layer of air on top. The mesh grid size is $4 \times 4 \times 4 \mu\text{m}^3$.

4.3. Results and discussions

4.3.1. Levelness of single-melt track

The levelness of the single-melt track was examined by employing simulation. The laser beam was considered as a simplified heat source moving from right to the left (see Figure 4.2) and the laser power was absorbed by the top surface of the powder bed. Figure 4.2(a) depicts the temperature distribution of single-melt track at cross-section $z = 130 \mu\text{m}$ at $t = 1300 \mu\text{s}$, where the white contour line encompasses the area where the temperature is above the liquidus temperature. Due to the applied heat source, metal powders near the laser spot were heated up

and started to coalesce together when they reached the melting point, giving rise to the formation of a melt track. When the temperature of the surface near the laser spot approached the boiling point, a keyhole was formed because of the recoil pressure as shown in Figure 4.2(a). Right after the laser beam moved away to the next position (or switched off), the keyhole collapsed due to the reversal motion of the liquid metal led by surface tension force. In addition, the geometry of the melt track is nonuniform, which can be attributed to the Marangoni force and recoil pressure. As depicted in Figure 4.2(b), the melt track is higher at the beginning of the scanning but becomes lower at the end of the scanning. The results are in good agreement qualitatively with previous simulation and experimental studies [54, 59, 118]. At the beginning of the melt track, molten material was pulled from the hot laser spot towards the cooler region due to the Marangoni effect and recoil pressure leading to an increased track height. On the other hand, due to the high cooling rate when the laser was switched off, and as the keyhole was not completely filled up, a recess was formed at the end of the melt tracks.

Figure 4.2: Temperature distribution of single-melt track at cross-section $z = 130 \mu\text{m}$ at (a) $t = 1300 \mu\text{s}$, (b) $t = 1500 \mu\text{s}$. The white contour line encompasses the area where the temperature is above the liquidus temperature. After the laser beam is switched off for $200 \mu\text{s}$ ($t = 1500 \mu\text{s}$), a recess can be observed at the end of the track.

4.3.2. Levelness of multi-melt track

Different scanning strategies such as parallel scanning, spiral scanning, paintbrush scanning and chessboard scanning were generated from sequential and boustrophedon scanning strategies. Therefore, multi-melt track simulations were performed using sequential and boustrophedon scanning strategies as illustrated in Figure 4.3. Sequential scanning represents a unidirectional

scan from right to the left with constant hatch spacing of $h_p = 100 \mu\text{m}$ (Figure 4.3(a)). In the boustrophedon strategy, the laser beam moves continuously from right to the left and from the left to the right with a constant hatch spacing of $h_p = 100 \mu\text{m}$ (Figure 4.3(b)). Due to the limitation of the computational resources, simulation work was only conducted for three tracks. Nonetheless, it is sufficient to study the melt pool geometry and the levelness of the melt track.

The melt track height was measured as the average height of the melt track at different cross-sections where the reference plane, which has the melt pool height of zero, is taken as the top surface of the substrate. The melt track heights of the first, second and third tracks of the sequential and boustrophedon scanning strategies were plotted in Figure 4.4. For sequential tracks, the melt pool heights are highest at the beginning and decrease towards the end of the track, as shown in Figure 4.4(a). As explained in section 4.3.1, such nonuniformity is caused by the Marangoni effect, recoil pressure and rapid solidification. Since unidirectional scanning was employed in the sequential strategy, all the single-melt tracks exhibit higher heights at the beginning and lower at the end of the tracks. As a result, sequential scanning pattern forms non-flat printed surface – highest at the beginning and lowest at the end of the track. In contrast, the boustrophedon strategy produced a flatter printed surface as shown in Figure 4.4(b). Furthermore, Figure 4.5 depicts the cross-section view at $x = 864 \mu\text{m}$ of the boustrophedon strategy at $t = 1320 \mu\text{s}$ showing the temperature distribution and the molten metal of the melt pool from the second track flowing to the first track. In addition, the white contour line encompasses the area where the temperature is above the liquidus temperature. As the laser beam moved continuously from right to the left and from left to the right, the molten material flowed continuously from the n^{th} track to the $(n-1)^{\text{th}}$ track (see Figure 4.5). Since the molten material flowed continuously from

the beginning of the n^{th} track to the end of the $(n-1)^{\text{th}}$ track, the fluid flow was able to fill up the recess. As a result, the boustrophedon method was able to produce a flatter printed surface. However, the melt track was highest at the beginning of the first track and lowest at the end of the last track due to the Marangoni effect, recoil pressure and rapid solidification.

Figure 4.3: Two scanning strategies namely, (a) sequential and (b) boustrophedon, with (i) the schematic of the scanning pattern and (ii) the top view of the fused zone, and $h_p = 100 \mu\text{m}$ is the hatch spacing.

The study has not examined the density of the printed part under different scanning strategies. Especially, the main scope in this study is to understand the melt pool dynamics under different scanning strategies. In the research, three scanned tracks were investigated with the length of each melt track was 800 μm and hatch spacing was 100 μm . It means that only a tiny area was examined. To investigate the density of the printed part, further examining of laser power, scanning speed, and layer thickness on the melt pool geometry and the collapse of the melt pool need to be studied. Therefore, it is not conclusive enough to give comments on the density. Regarding about the interface of metal/gas (it also can be called the printed track surface morphology), it has been investigated locally at the beginning and the end of the melt tracks. The printed track morphology with different hatch spacing have been published [131]. Thus, this work focused on the surface morphology at the beginning and the end of the melt track. The molten metal/solid metal interface has also been examined by Yan *et al.* [131]. Therefore, this study has not further investigated it. However, by employing different printing parameters, the density and gas/metal interface can be further examined in the future work.

Figure 4.4: Melt track height of the first, second, and third track of (a) sequential, (b) boustrophedon scanning strategies at different cross-sections along the x -direction.

Figure 4.5: Cross-section view at $x = 864 \mu\text{m}$ of the boustrophedon strategy at $t = 1320 \mu\text{s}$ showing the temperature distribution and the molten metal of the melt pool from the second track flowing to the first track. The white contour line encompasses the area where the temperature is above the liquidus temperature.

4.4. Conclusions

Different scanning strategies has been studied in both experiment and simulation. However, it is still lacking in understanding the melt pool dynamics under different scanning patterns. Moreover, different scanning lines can be generated from sequential and boustrophedon scanning strategies. The simplified heat source model was employed to investigate the melt pool behaviour due to different scanning strategies. Two common scanning strategies have been tested and they were the sequential and boustrophedon scanning patterns. The simulation results showed that sequential scanning strategy leads to a non-flat printed surface – highest at the beginning and lowest at the end of the track. Boustrophedon strategy, on the contrary, produces a flat printed surface.

CHAPTER 5: SIMULATION OF KEYHOLE-MODE MELTING IN SELECTIVE LASER MELTING USING RAY TRACING MODEL

This chapter describes a physics-based CFD model developed to simulate keyhole-mode melting in the SLM process. The heat source model mimicked the multiple reflections of the laser beam by using the Fresnel absorption function. The model emulated the fluid flow and heat transfer of keyhole-mode laser melting process, which was validated by single-melt track experiments. In addition, the simulation results showed that the melt pool dynamics of a well-deep keyhole is unsteady as compared to the medium-deep keyhole. Different modes of fluid flow, such as downward, bottom backward, clockwise, and top forward flow were observed in the well-deep keyhole melt pool. On the other hand, the melt pool dynamics of the medium-deep keyhole was more stable with two main modes of fluid flow including the downward and backward flow.

5.1. Introduction

In the SLM process, the process parameters will directly affect the melt pool geometry. The melt pool can be in conduction-, transient- or keyhole-mode as depicted in Figure 5.1 [82]. As employing the same laser power and scanning speed but using different laser spot sizes, different melt pool modes can be formed. When a large laser beam spot size of $95.8\text{ }\mu\text{m}$ was used, the melt pool is at conduction-mode (see Figure 5.1(a)), however, when a small laser spot size of $50.0\text{ }\mu\text{m}$ was used, a keyhole-mode melt pool is formed as depicted at Figure 5.1(c). The melt pool between the conduction- and keyhole-mode is known as the transient-mode (see Figure 5.1(b)) [82]. The depth to width ratio can also be used to define the conduction- and keyhole-mode of the melt pool. When the depth to width ratio of the melt pool is smaller than 0.5, a conduction-

mode melt pool is formed [163]. Meanwhile, the melt pool is in the keyhole-mode when the depth to width ratio becomes larger than 0.5 [164, 165]. For instance with a laser power of 100 W and laser scanning speed of 188 mm/s, the melt pool would be in conduction-mode in which the melt pool has a semicircular geometry. However at high energy density – with the same laser power of 100 W but laser scanning speed of 100 mm/s, the melt pool would be in keyhole-mode in which the melt pool depth is much deeper than the melt pool width [164]. Similarly, the melt pool can be considered as transient-mode when the ratio between the melt pool depth and melt pool width is in between 0.5 and 1.0 [82].

Figure 5.1: Melt pool geometry of SS316L SLM at (a) conduction-mode, (b) transient-mode, and (c) keyhole-mode [82].

Many experiments have validated the occurrence of keyhole-mode laser melting in the SLM process. Bertoli *et al.* carried out single-melt track experiments of the SS316L powder with different laser powers and scanning speeds [154]. The study found that the melt pool can occur in either conduction- or keyhole-mode. In addition, King *et al.* performed experiments to

determine the conditions under which keyhole-mode laser melting will occur for selectively laser melted SS316L [164]. However, it is difficult to investigate the dynamics of the keyhole-mode induced melt pool by employing experiments. Therefore, numerical simulations have been adopted to demonstrate the mechanisms and defects in the keyhole-mode. For instance, Tang *et al.* explained the mechanisms of the molten flow during keyhole-mode laser melting [148]. The molten flow around the keyhole is intense and unsteady, and due to the vortex at the rear part of the melt pool, bubbles which can lead to pores are formed. Furthermore, Tan *et al.* also explained the formation of spherical and elliptical pore shapes [66]. As the collapsing keyhole can capture the gas bubbles into the melt pool, and due to the effect of surface tension, it forms into spherical and elliptical pore shapes.

In fact, it is challenging to model the keyhole-mode laser melting that occurs during the SLM process. An adequate representation would require improvements to the model. Most simulation works assumed a constant absorption coefficient of the laser heat source [54, 59, 63]. However, as reported by Trapp *et al.*, the absorption coefficient is dependent on the laser power and scanning speed [156]. Therefore, the assumption of constant absorption coefficient becomes inadequate at some regions, especially when the melt track is in the keyhole-mode. Furthermore in reality, multiple reflections of the laser in the keyhole determine how the energy is actually transferred. However, most simulation works assumed only the top surface of the powders covered by the laser beam spot would be heated [54, 146]. Therefore, in the previous simulation studies of SLM, the heat source has not been represented adequately.

Generally, transient-mode and medium-deep keyhole-mode is desired in printing, as it gives rise to the bonding in between layers. Some applications such as aerospace industry require specific microstructure, and this can be produced by controlling the penetration of the keyhole-mode in the printed part. However, there is a lack of deep insight into the melt pool dynamics during keyhole-mode melting due to its high complexity. Therefore, this work aims to develop a ray-tracing model to simulate the multiple reflections of the laser rays in the keyhole-mode laser melting with high accuracy at different laser powers and scanning speeds. While the ray-tracing model has been widely employed in laser welding simulations [49, 158], only a handful of studies applied it in the simulation of the SLM process [166]. Using the ray-tracing model together with CFD, the mechanisms and dynamics of the keyhole-mode melting in the SLM process were studied. Furthermore, this model brings the possibility in predicting porosity formation observed in realistic experiments.

5.2. Simulation setup

The 3D computational domain had a dimension of $x \times y \times z = 1920 \times 600 \times 400 \mu\text{m}^3$, where gravitational force was along the y-axis. The simulation domain comprised a 400 μm -tall SS316L substrate, 75 μm -thick layer of SS316L powder bed, and a 125 μm -tall layer of air above the powder bed. The powder was assumed to be spherical in shape and followed the Gaussian distribution with the powder diameter ranging from 16 to 45 μm , with the mean powder diameter of 30.5 μm . The steps to generate the powder bed are described in section 3.1.4.1. The cell size was $4 \times 4 \times 4 \mu\text{m}^3$ in the model. The initial temperature of the domain was set at 300 K. In addition, the laser beam radius was set as 27.5 μm , which followed a Gaussian distribution with the distribution factor of two. This study employed the ray-tracing model of the laser beam where

the details can be found in section 3.3.2. In the simulation, after the laser was switched off, the cooling time of 200 μs was performed.

5.3. Results and discussions

5.3.1. Dynamics of keyhole-mode melting

The dynamics of the keyhole-mode melting is described in this section. While investigating the dynamics of the keyhole-mode melting, it was noticed that the dynamics of the melt pool was more complex during the intensive penetration. In this study, when the depth to width ratio of the melt pool was larger than 1.0, it was considered as in keyhole-mode. In addition, the depth to width ratios of different keyhole-mode melt pools are listed in Table 5.1. Furthermore, two types of keyhole-mode melting were investigated, namely the medium- and well-deep keyhole. In the conduction-mode, the melt pool depth is roughly similar to the focus laser beam diameter. However, in the keyhole-mode, the melt pool can be penetrated deeply from two to a few times of the focused laser beam diameter. As listed in Table 5.1, the melt pool depths were three times greater than the focused laser beam diameter when the depth to width ratio is above 1.5. Thus, the ratio of 1.5 was taken as a reference value to classify the two types of keyhole-modes. A melt pool was considered as medium-deep keyhole when the ratio of melt pool depth to melt pool width is ranged from 1.0 to 1.5. When the ratio of melt pool depth to melt pool width is above 1.5, it was considered as a well-deep keyhole. Two simulated samples C and K (see section [3.5.3](#)) at different energy densities of 81 and 162 J/mm^3 were adopted to investigate the melt pool dynamics at different keyhole-modes. Sample C was simulated using laser power of 300 W and scanning speed of 900 mm/s. A melt pool depth of 120 μm and width of 100 μm were formed,

therefore, sample C was represented as a medium-deep keyhole. Sample K which was simulated using laser power of 300 W and scanning speed of 450 mm/s formed a melt pool depth of 278 μm and a melt pool width of 100 μm . As the ratio of melt pool depth to melt pool width is 2.53, it is then considered as a well-deep keyhole.

Table 5.1: Depth to width ratio in keyhole-mode melt pools [154]

Laser power (W)	Scanning speed (mm/s)	Melt pool depth (μm)	Mean value of melt pool width (μm)	Depth to width ratio
100	150	150	144	1.04
100	200	126	117	1.08
200	400	159	125	1.27
500	1500	123	92	1.34
300	900	128	89	1.44
300	600	198	130	1.523
200	300	266	130	2.05
300	450	302	140	2.16
400	1000	197	71	2.77
500	1250	223	79	2.82
200	200	329	155	2.86
300	300	524	138	3.8
500	1000	289	71	4.07
400	800	220	52	4.23
400	600	380	72	5.28
500	750	362	62	5.84

Figure. 5.2 depicts the simulated temperature and velocity distribution of the medium-deep keyhole formed in sample C at the cross-section of $z = 200 \mu\text{m}$ at $t = 600 \mu\text{s}$. The red contour encompasses the area that has been melted, while the white contour encompasses the area which exhibits temperature larger than the liquidus temperature. The white arrows represent main flow modes in the melt pool. There exist two main dominant flow directions in the melt pool: (1) downward flow from the top surface to the bottom of the front wall of the keyhole (see arrow 1 in Figure. 5.2) due to the recoil pressure penetrating strongly into the substrate and (2) backward flow moving from the bottom of the keyhole opposite to the scanning direction (see arrow 2 in Figure. 5.2). As the recoil pressure penetrates into the substrate, the molten liquid is pushed to the tail of the melt track maintaining an opened large keyhole and keeping the distance between the front and rear wall of the keyhole at about $200 \mu\text{m}$. This large distance prevents the molten metal from the rear wall to flow back to the front to merge with the front keyhole wall. Therefore, this inhibits the formation of bubbles, which in turn reduces the formation of pores.

The melt pool dynamics in the case of well-deep keyhole (sample K) is more turbulent as depicted in Figure 5.3. The simulated temperature and velocity fields at cross-section of $z = 200 \mu\text{m}$ were captured at different timesteps. It shows that different molten directions including the downward, bottom backward, clockwise, and top forward flow can be observed. Such molten flows were also observed in the laser welding simulation carried out by Lin *et al.* [49]. Similar to the medium-deep keyhole, the downward flow in the front keyhole wall (see arrow 1 of Figure. 5.3(c)) is attributed to the recoil pressure. In addition, this recoil pressure also plays a role in pushing the molten metal from the keyhole moving in the opposite direction of the scanning

direction, forming the bottom backward flow as depicted in Figure. 5.3(a) and Figure. 5.3(c) (arrow 2). Nevertheless, as the keyhole is very deep, the molten metal can only accumulate at the top of the keyhole and flows downward back to the keyhole as observed in the Figure. 5.3(b). At the same time, the molten metal at the bottom of the keyhole continues to flow upward along the melt pool boundary under the effect of the recoil pressure. These two different metal flows enhance the generation of the clockwise flow [150]. As the clockwise flow (arrow 3) becomes prevalent as shown in Figure 5.3(c), it leads to a larger bulge forming at the top of the keyhole. This cycle of clockwise flow continues and as a result, the molten metal from the rear wall eventually flow to the front and merge with the front keyhole.

Figure 5.2: Simulated temperature and velocity distribution of the medium-deep keyhole-mode at the cross-section of $z = 200 \mu\text{m}$ at $t = 600 \mu\text{s}$ of sample C. The red contour represents the

area have been melted, while the white contour depicts the area which has the temperature larger than the liquidus temperature. The white arrows represent main stream flows in the melt pool.

Furthermore, the laser rays are entrapped at the bottom of the well-deep keyhole [167] due to its deep and narrow geometry. As such, the reflections of the laser rays occur mostly at the bottom of the keyhole resulting in a larger bottom and a narrower top as depicted in Figure. 5.2(c). At the same time, as the laser continues to scan, a top forward flow is formed as shown by arrow 4 of Figure. 5.2(c). As the surface tension force plays a role in preventing the formation of the keyhole, therefore, the surface tension force causes the molten metal to move forward to fill up the keyhole forming a top forward flow. Additionally, the clockwise flow induces the formation of bubbles. In many cases, bubbles that are caught in the liquid/gas interface can escape from the melt pool. However, some bubbles are unable to escape from the melt pool and they become pores when the melt pool solidifies.

Figure 5.3: The temperature and velocity distribution of the well-deep keyhole-mode at the cross-section of $z = 200 \mu\text{m}$, at (a) $t = 190 \mu\text{s}$, (b) $t = 270 \mu\text{s}$, and (c) $t = 980 \mu\text{s}$ of the sample K. The red contour represents the area has been melted, while the white contour depicts the

area which has the temperature larger than the liquidus temperature. The white arrows represent main stream flows in the melt pool.

5.3.2. Prediction of keyhole-induced porosity

Experiments were performed to examine the formation of the keyhole-induced pores in well-deep keyholes. The laser power of 300 W and scanning speed of 300 mm/s were employed to print a single-melt track of SS316L powder (size ranging from 20 to 53 μm) in SLM[®] 280 HL. During the printing process, the oxygen content inside the chamber was set at 0.2 % controlled by the argon gas. The $80 \times 80 \times 8 \text{ mm}^3$ SS316L substrate was used to print the single-melt tracks. A thin layer of powder was deposited on the substrate, and in both simulation and experiment, the powder thickness was set as 50 μm . The 1070 nm Yb fiber laser was focused to a nearly Gaussian beam with a diameter of 80 μm . The melt track with a length of 3 cm was printed on the substrate. Then, the substrate with the single-melt track was cut at different cross-sections using cutting machine Struers Discotom-10, and mounted for cross-section analysis. Metallographic grinding was performed with sand paper (320 CW, 600 CW, and 1000 CW) followed by automatic polishing using Struers Tegramin-25 with diamond suspension (9 μm and 3 μm), and finally, silica suspension (0.04 μm) was used for final precision polishing. In order to observe the melt pool geometry, etching is required, where Kroll's reagent etchant was applied. The microscope named Axioskop 2 was employed to visualize the melt pool geometry of the single-melt track.

In the experiment, the melt track was cut and measured at ten cross-sections. The average melt pool depths was $410 \pm 32 \text{ }\mu\text{m}$, and the average melt pool widths were $206 \pm 40 \text{ }\mu\text{m}$. The melt pool

geometry in the simulation was also measured at different cross-sections, and the average melt pool depths was $354.5 \pm 10 \mu\text{m}$, and the average of the melt pool widths was $179 \pm 9 \mu\text{m}$. The deviation between the simulation and the experiment is less than 15 %. Hence, the simulation result is consistent with the experiment. It was found that similar pore can be observed in the simulation as depicted in Figure 5.3. The pore is in a spherical shape and is consistent with the observations in ref. [148].

Figure 5.4: The observation of pore in the (a) experiment and (b) simulation with laser power of 300 W, scanning speed of 300 mm/s, and beam diameter of 80 μm .

Figure 5.5: Dynamics of examined bubble (a) at $t = 1770 \mu\text{s}$, (b) at $t = 1780 \mu\text{s}$, (c) at $t = 1950 \mu\text{s}$, and (d) at $t = 2150 \mu\text{s}$.

In this study, the boundary of melt pool and the solidified zone have been considered. The formation of the pore observed in the simulation in Figure 5.3 is illustrated in Figure 5.4. A bubble is first formed in the keyhole and is attempting to move out of the keyhole at $t = 1770 \mu\text{s}$ as depicted in Figure 5.4(a). The bubble then exists in the melt pool (Figure 5.4(b)) before it reaches the melt pool boundary at $t = 1950 \mu\text{s}$ (see Figure 5.4(c)). When the bubble reaches the melt pool boundary, it starts to solidify and becomes a pore as observed in Figure 5.4(d).

5.4. Conclusions

This work shares the computational model to simulate keyhole-mode melting in the SLM process. The simulation results elucidated the melt pool dynamics of the medium-deep keyhole and well-deep keyhole. One important finding of this work is that the model is able to reveal complex melt pool dynamics of the keyhole-mode, especially in the well-deep keyhole-mode. In fact, it is very challenging to observe by employing the experimental methods such as high-speed camera monitoring or X-ray CT analysis. However by improving the model including the laser heat source and the surface tension force, the complex physics of the melt pool is revealed. It brings the benefits in saving experimental and human resources to understand the physics in the SLM process. It shows that the well-deep keyhole exhibits unstable melt pool dynamics, causing the collapse of the keyhole and the formation of the bubble, which leads to pores. The molten flow, however, is more stable in the case of the medium-deep keyhole. Two main flows, downward flow at the front wall and backward flow at the rear keyhole, exist in the medium-deep keyhole, maintaining the stability of the melt pool. Hence, it prevents the formation of entrapped bubbles and reduces the appearance of pores. Furthermore, the model also adequately predicts the keyhole-induced porosity found in the solidified melt track.

CHAPTER 6: DISCONTINUITY OF OVERHANGING MELT TRACK IN SELECTIVE LASER MELTING

This chapter shares the findings of the formation of overhanging melt track in the SLM process. This was achieved by incorporating Fresnel reflections in the laser beam through the ray-tracing model. The CFD model was employed to investigate different overhanging situations, including perpendicular and parallel overhanging melt tracks on a cuboid block, as well as parallel melt tracks on an inclined block. The process parameters are found to strongly affect the surface morphologies of the overhanging melt track where discontinuities were observed. The subsequent defects caused by the discontinuity have also been investigated. Furthermore, the study also found that high laser power alleviates the discontinuity phenomenon of the overhanging melt track. However, by applying high laser power at high energy density, high value of melt pool depth was formed, causing warpage to the overhanging printed part. Nevertheless, employing high laser power while maintaining low energy density can eliminate phenomenon such as irregular pores, partially-melted powder, deep melt pool formation and geometrical inaccuracy.

6.1. Introduction

In the SLM process, overhanging structures with unsupported downward facing surfaces are unavoidable in the SLM process. Typically, different types of defects can be observed near the overhanging regions. One of the most common defects is warpage. According to Wang *et al.*, warpage becomes more prevalent as the number of processing layers increases [70]. This is due to the accumulation of heat that leads to residual stress buildup. The study also revealed that

longer scanning vectors result in more severe warpage as compared to short scanning vectors. Moreover, severe warpage would lead to the termination of the recoating process due to uneven powder bed [70]. In addition, dross formation is commonly found on the downward facing surface of the overhanging structures although with optimized volume energy density, for example between 60 and 80 J/mm³ for SS316L, they can be reduced [93]. Furthermore, shrinkage is also commonly observed at overhangs. Due to the changing density of the metal during repeated melting and solidification during the SLM process, it causes the printed part to shrink and hence resulting in geometrical inaccuracies [99]. Balling or discontinuous melt tracks are also often detected in overhanging structures and the resultant surface roughness can lead to porosity concentrations within as-fabricated samples [168, 169].

To achieve a better understanding of overhang printing in SLM, experiments have been conducted to explore the effects of printing parameters on the quality of the overhanging printed part. The effects of various parameters on warpage were tested in Wang's work [70]. According to their work, warpage becomes severe at a small inclined angle, or when printed at slow scanning speed and high laser power. Additionally, Covarrubias *et al.* investigated the roughness of the downward and upward facing surface in the overhang printing [94]. The study found that downward facing surface typically contained higher surface roughness than the one at the upward facing surface. Different methods were employed to improve the quality of as-printed parts with overhanging structures. DePond *et al.* investigated the effects of processing parameters on the defects caused by the overhangs [169]. The study found that large dross will occur when using high energy density, while balling will form when using low energy density. In addition, layer-to-layer scanning rotation strategies have a significant effect on surface roughness [169]. As the

number of printed layers is increased, the surface roughness of the top surface is increased when the scanning strategy with the rotation angle of 0° is applied. Likewise, the roughness remains almost unchanged if the rotation scanning strategy is employed. In addition, the effects of supporting structures on Ti-6Al-4V overhanging printed parts had also been investigated by Wang *et al* [170]. The study adopted solid gap support structure, where a support surface was put underneath the overhang and the gap between the support surface and the overhang was filled with unmelted metallic powder. It found that the microstructure and mechanical properties of the overhang were improved even though there are warpages by employing solid gap structure. On the other hand, the warping phenomenon can be alleviated by applying thin-wall tooth contact support structure although it will lead to lower Vickers hardness of the overhang. As a result, using solid gap supports with teeth at the tip-end in the overhanging printing was recommended.

Computational models were also used to investigate overhang printing and its related defects. FEM was adopted to study the overhanging melt pool behaviors at different inclined angles [171]. It was found that at small inclined angles, the melt pool shape would be irregular leading to melt pool instability. On the contrary, increasing the inclined angle will improve the quality of downward facing surface. Moreover, previous simulations on overhanging structures proved that balling effects could be alleviated by decreasing laser power and scanning speed [168]. Furthermore, a continuous overhanging melt track can be actualised by re-melting the overhanging location [168]. As observed in the simulated result, discontinuities had appeared after the first scanning. However, by repeating the scanning process on the same location a second time, the defect was eliminated.

Despite previous research works on various aspects of overhanging structures, the physical mechanisms of defect formation (e.g., discontinuity, porosity, unmelted/partially-melted powders within porosity) in overhang printing have not been fully understood. Therefore, this work aims to make use of powder scale simulation to investigate the formation mechanisms of discontinuous overhanging melt track. Physical origins of porosity and unmelted/partially-melted powders were also revealed. Furthermore, optimization of the processing parameters was also carried out to eliminate melt track discontinuities while achieving high geometrical accuracy. Last but not least, experiments were also performed to verify the simulation results.

6.2. Simulation setup

In order to simulate the overhanging melt track efficiently, a block of SS316L was modelled and it sits on the substrate. The block acts as already-melted and solidified powder. It also comes in different shapes and sizes – cuboid and 40°-inclined for different investigations as depicted in Figure 6.1. The inclined angle was formed between the downward facing surface and the z -axis. In addition, perpendicular printing and parallel printing are two common strategies in overhang printing [141]. Perpendicular printing is formed when the laser beam scans perpendicularly with respect to the block-powder interface (see Figure 6.1(a)). On the other hand, parallel printing is formed when the laser beam scans in parallel to and along the block-powder interface as seen in Figures 6.1(b) and (c). In this study, three types of overhanging part were employed: cuboid block for perpendicular printing, cuboid block for parallel printing and 40°-inclined block for parallel printing as depicted in Figure 6.1. Previous study found that severe defects such as dross and shrinkage are very common at low inclined angle such as 25° and 30° [70]. In order not to repeat the work that has been carried out and to investigate defects other than dross and shrinkage, this study proposes the investigation of defects at a 40°-inclined angle of which the results are

applicable to other inclined angles such as 50° and 60° . Similar to 40° -inclined angle, 50° - and 60° -inclined angle has one half of the melt track was printed on an inclined block with a thin thickness where below was full of powder. Moreover, choosing a larger angle such as 70° or 80° will be very similar to printing on a right-angled cuboid.

The DEM was first employed to model the powder bed. The dimensions of the model were $x \times y \times z = 3500 \times 1500 \times 600 \mu\text{m}^3$ and the dimensions of substrate, blade and blocks can be found in Figure 3.3 (see section 3.1.4.2). In this work, SS316L powder with diameters ranging from 20 to $53 \mu\text{m}$ was employed in both simulation and experiment. The powder was deposited on the block and a blade was then moved along the x -axis to form a uniform $50 \mu\text{m}$ -thick layer of powder as depicted in Figure 3.4 (see section 3.1.4.2). Next, the powders' radii and the coordinates were exported to OpenFOAM® [144] for the CFD simulation. The CFD model has a domain size of $x \times y \times z = 2560 \times 500 \times 400 \mu\text{m}^3$ in which the gravity is along the y -axis. The schematics of the CFD simulation domain using three different types of blocks are shown in Figure 6.2. The simulation domain comprised a $300 \mu\text{m}$ -tall block, $50 \mu\text{m}$ -thick layer of powder bed and a $150 \mu\text{m}$ -tall layer of air above the powder bed. In order to save computational costs, the substrate was not included in the CFD model (as shown in Figure 6.1) since in single overhanging melt track, the heat transfer and melting process occurs at a small region around the block and the powder bed. In the CFD model, the cell size was $4 \times 4 \times 4 \mu\text{m}^3$ and the initial temperature of the domain was set at 300 K. In addition, the laser beam diameter was set as $80 \mu\text{m}$, which follows a Gaussian distribution with a distribution factor of two where the multiple reflections of laser were simulated by applying the ray-tracing model (see section 3.3.2).

Figure 6.1: Schematics of powder bed containing overhanging feature of (a) perpendicular printing on cuboid block, (b) parallel printing on cuboid block and (c) parallel printing on 40°-inclined block.

Figure 6.2: Schematics of CFD simulation domain of (a) perpendicular overhanging printing on cuboid block, (b) parallel overhanging printing on cuboid block, and (c) parallel overhanging printing on 40°-inclined block.

The printing parameters used for the simulation of the overhanging melt tracks on different blocks mimicked that of the experiment's listed in Table 6.1. Samples A, B and C were simulated

employing the same laser power of 120 W and scanning speed of 800 mm/s on cuboid and inclined blocks with perpendicular and parallel scanning directions. This first group of testing was performed to observe other defects instead of dross and shrinkage that happened in overhangs. The second group of testing involved samples C, D and E where the impact of laser powers on the overhanging melt track morphologies were investigated. Next, the third group of testing examined how varying laser powers and scanning speeds, while keeping the energy density constant (samples C, F and G), influence the overhanging melt tracks.

Table 6.1: Printing parameters of overhang samples

Sample	Laser power (W)	Scanning speed (mm/s)	Scanning direction	Block	Energy density (J/mm ³)
A	120	800	Perpendicular	Cuboid	37.5
B	120	800	Parallel	Cuboid	37.5
C	120	800	Parallel	40°-inclined	37.5
D	200	800	Parallel	40°-inclined	62.5
E	240	800	Parallel	40°-inclined	75.0
F	60	400	Parallel	40°-inclined	37.5
G	180	1200	Parallel	40°-inclined	37.5

6.3. Experiment setup

In the experiment, SLM[®] 500 HL was used to carry out the printing of samples with overhanging structures. The machine uses Nd:YAG laser with a beam diameter of 80 μm . In the experiment of overhang printing, the inclined angle was formed between the downward facing surface and the z-axis. Previous studies have shown that severe dross and shrinkage will occur at low inclined angles of 25° to 30° [70]. Fortunately, by orientating the 3D model before printing, low inclined angles can be avoided [172]. Therefore similar to the simulation, in this experimental study, samples were printed on a 40°-inclined block to prevent dross and shrinkage as mentioned in section 6.2. Moreover, in the investigation of overhanging melt track morphology, the parallel printing of the overhanging melt track on the 40°-inclined block could be revealed clearer as compared to the parallel printing of the overhanging melt track on a cuboid block. Thus, the parallel printing of overhanging melt track on cuboid block was not experimentally performed. In addition, Kruth *et al* found that the first layer of overhanging structure in both perpendicular and parallel printing were commonly broken [98]. Hence, it hindered the observation of melt track morphology. As a result, the experiment of the perpendicular printing of overhanging melt track on cuboid block was also not carried out. The processing parameters including laser powers and scanning speeds of overhang printing on the 40°-inclined block can be found in Table 6.1. All the samples were printed using the boustrophedon scanning strategy with hatch spacing of 80 μm and powder layer thickness of 50 μm [146]. During the printing process, the oxygen content inside the chamber was set to 0.1 %. After the samples were printed, they were hot mounted and polished, and investigated on their melt-track geometry, melt pool depth, the unmelted powders, partially melted powder and pores.

6.4. Results and discussions

6.4.1. Observation of discontinuity in overhanging melt track

Figure 6.3 shows the simulation results of various overhanging melt tracks of samples A, B and C of which the same laser power (120 W) and scanning speed (800 mm/s) were used. Sample A was printed with the laser scanning perpendicular to the cuboid block, sample B was printed with the laser scanning in parallel to cuboid block and sample C was printed with the laser scanning in parallel to the 40°-inclined block. The laser center was located at the position of $z = 200 \mu\text{m}$.

From the simulations, one common defect observed was the discontinuities in the overhanging melt tracks. As noticed in Figure 6.3(a), the printed melt track is continuous on the cuboid block. However, there is discontinuity when the melt track was printed on a thick powder bed, and the thickness was seven times of the one-layer thickness in the simulation. In addition, the discontinuity can also be observed in sample B where one half of the melt track was on the block and the other half was on the powder as shown in Figure 6.3(b). Moreover, the discontinuity was also observed in sample C (see Figure 6.3(c)). In sample C, the laser center was located at $z = 200 \mu\text{m}$ where the block has a thickness of $42 \mu\text{m}$ as depicted in Figure 6.1(c)(ii). As a result, one half of the sample C melt track was printed on an inclined block where the thickness is less than $42 \mu\text{m}$ and below which was full of powder. In addition, one side of the overhanging melt track which was printed on the powder-supported zone (see Figure 6.2(c)) could be considered as printing on a thick powder bed. As noticed from different overhanging structures, the overhanging melt track morphologies on large layer thickness of powder were different compared to the melt tracks fully printed on the block with low layer thickness of $50 \mu\text{m}$. Therefore, the large thickness of powder has a significant effect on the overhanging melt track

morphology. Previous studies found that surface tension [57] and contact angle [173] play important roles in forming balling or discontinuous melt track. In sample A, the maximum temperature of the melt pool when the laser is at the block-supported zone and at the powder-support zone were 3650 K and 3732 K respectively. Therefore, the surface tension at block-supported zone and powder-supported zone can be considered as similar. In samples B and C, the maximum temperature at block-supported zone and powder-supported zone were almost the same, therefore, similar surface tension values were also generated. Thus, contact angle has a significant effect leading to discontinuities in overhang printing. In addition, when the material of the molten flow and the substrate or block are similar, the contact angle would be mainly dependent on the surface roughness of the substrate or block [174, 175]. During the printing process, a uniform contact angle could form at block-supported zone, hence, it enhances the formation of uniform melt track. However, as the powder-supported zone exhibits high surface roughness in the range of the powder diameters (20 to 53 μm), irregular contact angles were easily formed at different cross-sections. This leads to the formation of irregular overhanging melt tracks at the powder-supported zone. Furthermore, the packing density of the powder bed, which is the ratio between the volume of powder particles and the total volume of powder bed, could affect the melt pool geometry [57]. The melt pool is uniform and well-defined at higher packing density, while an irregular melt pool will be formed at low packing density. Therefore, an irregular/discontinuous melt track could easily occur in overhang printing as the packing density of the powder-supported zone is lower than one of the powder bed on the block.

Figure 6.3: Simulated melt track morphologies of sample (a) A, (b) B, and (c) C where (i) indicates cross-section at $x = 1050 \mu\text{m}$ and (ii) represents the top-view of the melt track.

In the experiment, samples A and B were not printed as explained in the section 6.3. Sample C was fabricated to validate the morphology of the melt track due to parallel printing on the 40° -inclined block. Figure 6.4(a) shows the geometry and dimension of the designed part. Following the simulations, laser power of 120 W and laser scanning speed of 800 mm/s with hatch spacing of $80 \mu\text{m}$ were employed to print the sample. With the help of a laser digital microscope (Keyence VK-X200), the morphology of the overhanging area of this experimental sample was captured as shown in Figure 6.4(b). It is observed that the experimental result also exhibits discontinuities at the overhanging melt track. Figure 6.4(c) shows the contour of the simulated melt track at the

overhanging regions which concur well with the fabricated overhanging melt track in Figure 6.4(b).

Figure 6.4: Schematic of (a) the design of the overhanging part with an inclined angle of 40° , and morphology of the (b) examined area viewed from the top, and (c) simulated overhanging melt track of sample C viewed from the top.

This chapter used the ray-tracing model which has been validated in the Chapter 3, section 3.5. Therefore, in the overhanging melt track simulation, the quantitative comparison of the melt pool geometry between the simulation and the experiment have not been considered. In the study, the melt track morphology viewed from the top is mainly used to validate the simulation result. In fact, to compare to the simulated melt track morphology to the experimental one is much more difficult, requiring the accuracy in the surface tension force and laser heat source. That is the reason the simulation of humping in SLM is recent published even though it has been reported for a period of time in the experimental studies.

6.4.2. Defects due to discontinuous overhanging melt track

When the discontinuous overhanging melt track is formed, the bonding in between two layers and two adjacent melt tracks are poor. Furthermore, discontinuous overhanging melt track affects the surface roughness of the subsequent layers. Therefore, it can easily lead to other defects such as pores or partially-melted powder. A simulation was performed to confirm the existence of these defects. After the first melt track of sample C has solidified, the geometry of the top surface was exported as a STL file. This STL file was then exported to the DEM model and it also served as a boundary surface in the y -axis (see Figures 3.6(a-c)). After that, a second layer of powder was deposited on top of the STL surface which was representative of the first melt track (see Figures 3.6(d-f)). As the surface of the first melted layer was uneven with peaks and valleys, it resulted in the second layer having a non-constant thickness at different points even though its surface is flat as shown in Figure 6.5(a). The second layer of powder was melted by applying the laser heat source at $z = 200 \mu\text{m}$. In addition, the morphology of the second layer of the melt track at cross-section of $z = 230 \mu\text{m}$ is depicted in Figure 6.5(b). Many irregular pores and partially

melted powder particles can be observed in the simulated melt track as seen in Figure 6.5(c) which is an enlarged view of Figure 6.5(b).

An experiment was carried out to verify the results obtained in the simulation. In the experiment, laser power of 120 W and scanning speed of 800 mm/s with hatch spacing of 80 μm were applied. The samples were polished on the yz -plane to reveal the irregular pores and partially-melted powder in the overhanging melt track. Metallographic grinding was performed with sandpaper (320 CW, 600 CW, and 1000 CW) followed by automatic polishing using Struers Tegramin-25 with diamond suspension (9 μm and 3 μm) and silica suspension (0.04 μm). In this work, n was employed to keep track of the layer number and n begins from 0. To observe the partially melted powder in between two layers – $(n+1)^{\text{th}}$ layer and $(n+2)^{\text{th}}$ layer, the melt pool was etched for ten minutes by applying Kroll's reagent etchant. Figure 6.5(d) reveals irregular pores and partially melted powder that were found in between the layers. As noticed, some of the melt pools at $(n+1)^{\text{th}}$ layer has a small portion of solidified metal (see Figure 6.5(d)). As the melt tracks were discontinuous, the melt pools along the x -axis were irregular, where some regions had a small portion of solidified metal. Hence, it leads to a large gap in between the $(n+1)^{\text{th}}$ layer and $(n+2)^{\text{th}}$. As such, powder particles can be trapped inside the gap, resulting in uneven layer thickness of the subsequent layer. Furthermore, applying the same energy density on areas where the powder bed is thick due to the valleys in the previous melt track may not produce sufficient energy to fully melt all the powders. As a result, irregular pores and partially melted powder were formed as observed in both simulation and experiment. It is true that the irregular pores and the unmelted/ partially-melted powder can be found in general SLM printing. However due to the

discontinuities in overhanging melt track, it gives rise for the formation of irregular pores and the appearance of unmelted/partially-melted powder.

Figure 6.5: Simulated morphology of (a) deposited powder bed which was recoated on top of the melt track at $(n+1)^{\text{th}}$ layer, (b) melt track at $(n+2)^{\text{th}}$ layer using the processing parameters for the melt track at $(n+1)^{\text{th}}$ layer, (c) melt track at $(n+2)^{\text{th}}$ layer using the processing parameters for the melt track at $(n+1)^{\text{th}}$ layer, (d) melt track at $(n+2)^{\text{th}}$ layer using the processing parameters for the melt track at $(n+1)^{\text{th}}$ layer.

sample C at cross-section of $z = 230 \mu\text{m}$ after the melt track has been cooled down for $300 \mu\text{s}$ where pores and partially-melted powder were captured, (c) enlarged view of (b), and (d) irregular pores and partially-melted powder in between two layers found in the experiment. In the simulation, $n = 0$.

6.4.3. Influence of high laser power on overhanging melt track

To investigate the influence of laser power on the discontinuities in overhanging melt track, simulation was performed using the same scanning speed of 800 m/s and different laser powers of 120 W , 200 W and 240 W . Figure 6.6 shows the simulated melt track morphology of the overhanging melt track printed on the 40° -inclined block of sample C, D and E (see Table 6.1). Sample C that used a low laser power (see Figure 6.6(a)) exhibits a high number of discontinuities. On the other hand, samples D and E which used high laser powers resulting in higher energy densities, display fewer discontinuities as shown in Figures 6.6(b) and (c). According to previous studies, the discontinuous melt track is closely related to the contact angle [83, 176]. For instance, the melt track was easily broken into droplets at high contact angle, while a smooth and continuous melt track could be easily formed at a low contact angle [83]. In addition, Yadroitsev *et al.* discussed the influence of Plateau-Rayleigh instability on the continuity of the melt track [83]. The study found that when a large melt pool width is formed, it enhances the stability of the melt track. As a melt track produced by high laser power produces a larger melt pool width, therefore, the overhanging melt track printed with higher laser power has a lower frequency of discontinuities. On the other hand, Hu *et al.* found that driving forces, especially surface tension gradient and recoil pressure, play an important role in contact angle evolution, and as a result, affecting the melt track morphology [177]. In the simulated overhanging melt track, the

maximum temperature of the melt pool in sample C, D and E during the melting process were 3600K, 3900 K and 4050 K respectively. Hence, the temperature gradient of sample E printed with higher laser power (240 W) was larger than the ones of samples C (120 W) and D (180 W). Consequently, sample E also exhibited a larger surface tension gradient in the melt pool as compared to that of samples C and D. Moreover, surface tension gradient or Marangoni force plays a role of delivering molten material from the center to the edges of the melt pool and from the keyhole to the rear along the longitudinal direction [63, 177]. As a result, the molten metal was spread steadily and filled up some discontinuities and therefore producing a more continuous melt track. In addition, by employing high laser power on sample E leads to a deeper melt pool due to the higher recoil pressure. As a deep melt pool has higher wettability, it improves the continuity of the overhanging melt track. Furthermore, the lifetime of the melt pool was also considered. The lifetime of a melt pool was estimated from the time when the material was melted until it was fully solidified. As such, melt pools with deeper melt pool depth and higher maximum temperature would have a longer lifetime [177]. According to the simulation results, at the cross-section of $x = 1000 \mu\text{m}$, samples C, D and E had a lifetime of 640 μs , 910 μs and 1060 μs respectively. The long lifetime of sample E allows and enhances the spreading of molten metal and as a result reduces the frequency of discontinuities. Therefore, by employing high laser power, high surface tension gradient and longer lifetime of the melt pool were exhibited. These lead to the reduction of discontinuities. Unfortunately, using high laser power together with high energy density results in the formation of a large melt pool as seen in Figures 6.6(b)(i) and (c)(i) which is non-desirable.

Figure 6.6: Simulated melt track morphology of sample (a) C, (b) D, and (c) E where (i) indicates cross-section at $x = 900 \mu\text{m}$, and (ii) represents the top-view of the melt track.

The melt pool geometry of samples C and E were investigated experimentally. The samples were chosen as sample C uses the lowest laser power and sample E uses the highest laser power. The geometries of the samples are shown in Figure 6.4(a). In order to observe the melt pool geometry, Kroll's reagent etchant was applied to the polished samples for ten minutes. Figure 6.7(a) shows that the geometry of sample C is close to the designed geometry with an accuracy of more than 95% for both the designed angle and overhanging height. On the contrary, by applying high laser power, large deviations (30 to 40%) of the overhang height and designed angle were observed in sample E (see Figure 6.7(b)).

Furthermore, the melt pool geometry in Figure 6.7 shows that when higher laser power is employed (sample E), deep melt pools will be formed at the overhanging regions (see red contour). It shows that some of the melt pools are two times deeper than those at the solidified cuboid block (see Figure 6.7(b)). Moreover, sample E has higher maximum temperature (4050 K) which results in higher temperature gradient. This leads to larger thermal stress accumulation at the solidified overhanging melt track and consequently results in warping. On the contrary, at low laser power, the melt pools at the overhanging regions are similar to those at the solidified cuboid block (see Figure 6.7(a)). Additionally, sample C had a lower maximum temperature of the melt pool (3600 K) leading to a lower temperature gradient. As a result, a small amount of thermal stress was generated which leads to less warpage.

The study found that higher laser power can alleviate discontinuity at the overhanging melt track. However, by employing high laser power with high energy density, the maximum temperature of the melt pool increases and that results in high thermal gradient. As higher thermal gradient is formed, warpage occurs and leads to geometrical inaccuracy of the overhanging printed part. As a result, using high laser power together with high energy density is not suitable to achieve high geometrical accuracy while alleviating the discontinuities at the overhanging structures.

Figure 6.7: Overhanging melt pool geometry of sample (a) C and (b) E

6.4.4. Behaviour of overhanging melt track by employing high laser power while maintaining low energy density

In overhang printing, a conduction-mode or transient-mode melt pool can reduce geometrical inaccuracies. Additionally, a shallow melt pool depth can only be formed by applying low energy density. However, at low energy density, a small melt track width or a discontinuous melt track can easily occur. In addition, discontinuous melt track leads to pores and partially-melted powder. Therefore, it is important to optimize the processing parameters to produce a conduction- or transient-mode melt pool while alleviating the discontinuities at the overhanging melt track. It has been shown that using the same energy density generates similar melt pool geometries, in

which higher laser power produces deeper and wider melt pool [154]. Furthermore, the melt pool depth and width of sample C at cross-section of $x = 900 \mu\text{m}$ was 48 and $104 \mu\text{m}$ respectively. Thus, a conduction-mode melt pool was formed in sample C as seen in Figure 6.6(a)(i). In addition, sample C produced the inclined angle and the overhanging height of the solidified cross-section closely to the desired geometry. Therefore, simulations were performed to investigate the effect of the laser scanning speed and laser power while maintaining the same energy density that was used in sample C. Three samples C, F and G were investigated with the laser powers and scanning speeds listed in Table 6.1.

Figure 6.8 depicts the melt track morphology of samples C, F and G. It shows that at lower scanning speed, a continuous melt track was formed as depicted in Figure 6.8(b). This similar phenomenon was also observed in previous study [168]. In comparison to sample C in which the melt pool had a lifetime of $640 \mu\text{s}$, sample F which was simulated at lower scanning speed produced a melt pool with a longer lifetime of $750 \mu\text{s}$. Therefore in sample F, the molten metal has longer time to flow to the surrounding area resulting in a continuous melt track. However, as low laser power was employed in sample F, the melt track width is much smaller as compared to that of samples C and G (see Figures 6.8(a) and (c)). On the other hand, the melt pool of sample G had the shortest lifetime of $510 \mu\text{s}$. It also produced the highest maximum temperature (4150 K), while samples C and F had a lower maximum temperature of 3600 K and 3400 K respectively. It means that sample G had higher surface tension gradient. Hence, a stronger Marangoni flow was formed in the melt pool of sample G, enhancing the spreading of the molten metal. As a result, sample G (see Figure 6.8(c)(ii)) produced a smaller number of discontinuities compared to sample C as depicted in Figure 6.8(a)(ii).

Figure 6.8: Simulated melt track morphology of sample (a) C, (b) F and (c) G where (i) indicates cross-section at $x = 900 \mu\text{m}$ and (ii) represents the top-view of the melt track.

To further examine the contour of the melt track, an experiment was performed. The geometry and dimension of the designed part is shown in Figure 6.4(a). With the help of a laser digital microscope named Keyence VK-X200, the morphology of the examined overhanging area of this experimental sample was captured and shown in Figure 6.9. It was found that by employing the processing parameters (lower laser power and scanning speed) of sample F, it enhances the formation of a continuous overhanging melt track as seen in Figure 6.9(b). Similarly, by increasing the laser power and scanning speed, the contour of the melt track would also be

continuous (see Figure 6.9(c)). Therefore, using high laser power while maintaining low energy density can alleviate the discontinuities at the overhanging melt track.

In addition, Figure 6.10 depicts the cross-section of the overhanging melt tracks from samples C, F and G whose geometries are close to the designed part with deviation lesser than 5%. However, the printed melt track of sample F is porous as shown in Figure 6.10(b). This was because of the narrow melt track width (Figure 6.9(b)(i)), which results in a lack of bonding in between the layers and in between the adjacent melt tracks. Sample G, however, was fabricated using a higher laser power. Therefore, the printed part exhibited deeper and wider melt pool, which produces better bonding between the layers and between the adjacent melt tracks, along with high density and high geometrical accuracy as seen in Figure 6.10(c). Furthermore, the frequency of discontinuities was reduced as recorded in Figure 6.9(c).

Due to some unforeseen situations, the powder with different sizes were not able to order. Therefore, experiment with fine powder was not performed, and the simulated results of overhanging melt track with different powder sizes have not been validated. In addition, by applying different laser powers and scanning speeds while using the same powder, the discontinuities can be reduced. Therefore, the effect of powder sizes has not been further investigated. However, the effect of powder sizes on the discontinuities of the overhanging melt track still can be further examined in my future work.

Figure 6.9: Morphology of the examined overhanging area of (a) sample C, (b) sample F and (c) sample G viewed from the top. The designed printed part is shown in Figure 6.4(a).

Figure 6.10: Geometry of overhanging melt track of samples (a) C, (b) F and (c) G.

6.5. Conclusions

As investigated in the overhang printing, discontinuities at the melt track can be observed in both simulation and experiment. This leads to other defects such as lacking in bonding between layer and adjacent melt track. It is hardly to find the research work discussing about the discontinuities in the overhanging melt track in both simulation and in the experiment. On the one hand, employing high laser power at high energy density reduces the discontinuities found in the overhanging melt track but deep melt pool will be formed causing geometrical inaccuracy and defects such as warpage. On the other hand, with low laser power, geometrical accuracy of the overhanging melt track is vastly improved albeit with irregular pores and partially-melted powder. Thus, by employing low energy density at high laser power, the discontinuity of the overhanging melt track can be alleviated. Furthermore, it relieves phenomena such as irregular pores, partially-melted powder, deep melt pool formation, and geometrical inaccuracy.

CHAPTER 7: CONCLUSIONS AND FUTURE WORK

7.1. Conclusions

AM has garnered increasing attention in a wide range of applications, due to its ability to fabricate complex shapes directly from a digital file and without the need for additional tooling. Among several AM methods, the PBF process has attracted much interest due to its flexibility. One such process is known as SLM in which laser is employed as an energy source to selectively scan and melt the metal powders following to the cross-section of the part obtained from the digital file.

SLM is a highly complex multi-physics process. During SLM, the melting and solidification process has a significant impact on the mechanical properties of the printed part [16]. Therefore, it is valuable to predict the influences of the processing parameters on the resulting properties.

This work presents the successful application of DEM and CFD models in simulating the SLM process. The deposition of the powder bed is achieved by employing the DEM model. In addition, the CFD model was employed to mimic the complex physics of the SLM process, including heat and mass transfer, fluid dynamics, phase-change and laser-powder bed interaction. Furthermore, different forces such as Marangoni force, recoil pressure and surface tension, were considered in the model. Hence, the CFD model is able to adequately simulate real physics in the SLM process. Additionally, two models of the laser beam were proposed. Firstly, the laser beam was simulated as a simplified heat source applied on the top surface of the powder bed. It was found that this model is suitable to simulate the melt track in the conduction, transient and medium-deep keyhole

mode. On the other hand, the ray-tracing model, which is able to imitate the multiple reflections of the laser rays, performs remarkably with high accuracy in simulating well-deep keyhole. In addition, the multiple reflections in thick powder bed such as the powder bed containing overhanging features could be well-mimicked by employing the ray-tracing model. Furthermore, by using the ray-tracing model, the velocity field could be obtained adequately.

In this study, the simplified heat source model has been employed to investigate the influence of scanning strategies on the levelness of the melt track. Although, the multi-track has been examined by both simulation and experiment [54, 131], the influence of the scanning strategies on the melt pool dynamics has not been sufficiently investigated. In this work, an attempt is made to investigate the influence of the scanning patterns on the melt pool dynamics by using CFD to represent the melting and solidification process of SS316L powder during the SLM process. The aims of this work are to observe the levelness of printed surface based on different scanning strategies. Two common scanning patterns were tested: sequential and boustrophedon. The study found that sequential scanning strategy leads to a non-flat printed surface, while boustrophedon strategy produces a flat printed surface. The boustrophedon strategy is able to produce flat printed surface due to the formation of the molten flow flowing from the beginning of the n^{th} track to the end of the $(n-1)^{\text{th}}$ track. Thus, the recess appearing at the end of $(n-1)^{\text{th}}$ track can be filled up with molten metal. As the recesses at the end of each melt track (except the last melt track) are filled up, a flat printed surface is produced.

In addition, the study also investigated the melt pool dynamics in the keyhole-mode in SLM process. While studies have been performed on the melting process of SLM, there is a lack of deep insight into the melt pool dynamics during keyhole-mode melting due to its high complexity. Using the ray-tracing model together with CFD, the mechanisms and dynamics of the keyhole-mode melting in the SLM process were studied. Two keyhole-modes were investigated, namely medium-deep keyhole and well-deep keyhole. The simulation results showed that the melt pool dynamics of the well-deep keyhole is unsteady as compared to the medium-deep keyhole. Different modes of fluid flow, such as downward flow, bottom backward flow, clockwise flow and top forward flow are noticed in the well deep keyhole melt pool. On the other hand, the melt pool dynamics of the medium-deep keyhole is more stable with two main flows of downward and backward flow. Furthermore, the model brings the benefit of predicting the keyhole-induced porosity within the solidified track.

Last but not least, the overhanging melt track has been investigated by employing the ray-tracing model. In overhang printing, the formation of defects such as discontinuity, porosity and unmelted/partially-melted powders within porosity has not been fully understood. Therefore, this work aims to make use of powder scale simulation to investigate the formation mechanisms of discontinuous overhanging melt track. Physical origins of porosity and unmelted/partially-melted powders were also revealed. The study found that by employing high laser power, the discontinuity of the overhanging melt track can be alleviated. However by employing high laser power at high energy density, deep melt pool was formed. It leads to a high thermal gradient in the melt pool causing defects such as warpage and geometrical inaccuracy. On a contrary, although low laser power can produce high geometrical accuracy in overhanging melt track, it

leads to the formation of irregular pores and the presence of partially-melted powder. Fortunately, employing high laser power while maintaining low energy density can alleviate phenomenon such as irregular pores, partially-melted powder, deep melt pool formation and geometrical inaccuracy.

7.2. Future work

7.2.1. Widespread CFD model application

The CFD model opens opportunities to employ the model in different applications. Initially, SS316L was adopted to validate the CFD model as SS316L is one of the most investigated material in SLM [21]. Thus, the information of material properties, melt track morphology and defects could easily be found in both simulation and experiment. Then, it can be used to validate the CFD model. Indeed, the CFD model is able to apply to all types of metals and alloys. Especially, the model brings a majority benefit for high-cost alloys such as titanium alloys and Inconel alloys. Thus, the model will be further employed to optimize the processing parameters of SLM using high-cost alloys.

Another area of future work would be to improve the model such that is able to simulate the thermal stress and predict the formation of cracks in the as-printed part. By calculating the temperature gradient field in the CFD model, the thermal stress and cracks can be further predicted. As the CFD model was employed to simulate the multi-melt track and multi-layer, the thermal history in between the melt tracks and in between the layers could be revealed. Thus, the thermal stress and cracks analysis will be examined in future work. Although the CFD model

is in the mesoscopic scale, it is sufficed to optimize the processing parameters to avoid the formation of crack.

In addition, by coupling the phase-field model with the CFD model, the microstructure evolution can be adequately simulated. Takaki *et al.* modelled the crystal evolution at different temperature gradients where constant values were applied [178]. However, the temperature gradient in the SLM process depends on time-step, coordinates and processing parameters. This temperature gradient can be adequately computed by employing the CFD model. Thus in future work, the phase-field model could be coupled with the CFD model to simulate the microstructure evolution during the SLM process.

7.2.2. Building the CFD-DEM model

An important part of this study is to couple the DEM model with the CFD model. As of now, the DEM and CFD models can separately solve problems such as heat transfer and phase-change process respectively. The goal, however, is to generate a CFD-DEM model which can simulate melting, solidification processes, and the movement of powder concurrently. In every time-step, the model would be updating the information of particles' positions and velocity. As such, the model could calculate the interaction between the powder particles and the fluid flow [136]. By applying this model, it is possible to simulate the spattering of powder during the melting process and the attraction of powder particles to the melt pool [63]. This enhances the actual physics and the accuracy of the model.

In addition, a pressure of 12 mbar is set in the SLM chamber during the printing process. The simulation of powder bed inside the chamber can be achieved by employing CFD-DEM model where the pressure of the chamber is added. The pressure inside the chamber plays a role of improving the packing density of powder bed and avoiding the floating of the powder particles. Thus, the accuracy of the powder bed can be improved by applying pressure of the chamber in the CFD-DEM model.

7.2.3. Multi-shaped powder bed

Previous studies found that the SLM powders manufactured with different technical processes have various shapes [179]. By employed plasma rotating electrode process (PREP) a perfect spherical with smooth surfaces were produced [179]. On a contrary, water atomization (WA) process produces irregular shapes of powder [180]. In future, the different shapes of powder – not only spherical particles but also irregular particles, could be investigated. In order to simulate non-spherical particles, the overlapping multi-sphere model would be employed [139]. This allows the interactions among non-spherical particles to be rationalized as that of spherical particles.

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