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Multiple Material Additive Manufacturing Platform

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School of Mechanical and Aerospace Engineering

2019

Multiple Material Additive Manufacturing Platform

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School of Mechanical and Aerospace Engineering

A thesis submitted to

Nanyang Technological University

In partial fulfilment of the requirements for the degree of

Doctor of Philosophy

2019

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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31/07/2019.

Date

Assoc Prof Tran Anh Tuan

Authorship Attribution Statement

This thesis contains material from 2 papers published in the following peer-reviewed journal(s) / from papers accepted at conferences in which I am listed as an author.

Chapter 4 is published as Tan, J.L., Tang, C. and Wong, C.H., 2018. A Computational Study on Porosity Evolution in Parts Produced by Selective Laser Melting. Metallurgical and Materials Transactions A, 49(8), pp.3663-3673.

Chapter 4 is published as Tan, J.L., Tang, C. and Wong, C.H., 2018. Study and modeling of melt pool evolution in selective laser melting process of SS316L. MRS Communications, 8(3), pp.1178-1183.

The contributions of the co-authors are as follows:

- Assoc Prof Wong Chee How provided guidance during the development of the model.
- Dr. Tang Chao provided assistance to the writing of the codes.
- I performed the writing of the codes and analysis of the simulations.
- I am in charge of the writing and revisions of the manuscripts.

31 July 2019

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Date

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Tan Jie Lun

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Abstract

Additive manufacturing (AM) has brought about many benefits in the world of manufacturing. Its ability to construct parts with complex geometries, which was once impossible using the traditional manufacturing methods, allows for a great degree of design freedom.

Selective laser melting (SLM) is an AM technique which uses a powder-bed platform to build up parts layer by layer. The built parts are able to achieve near full densities compared to the traditional manufacturing methods. SLM uses a laser beam to fully melt the powder on the top layer, after which a new layer of powder will be deposited over the previous layer. Current SLM machines use single material for each print job due to their unique material deposition method. Unfortunately, the use of single material in each print job greatly limits the capabilities of SLM in expanding beyond their current applications since the mechanical properties are limited to the material used in the print. By allowing multiple materials in SLM, the desired mechanical properties can be varied within the part.

Numerical modelling has been used to study laser melting processes such as laser welding and SLM. The main advantages of using numerical modelling is that it allows numerous simulations to be conducted simultaneously and avoids material wastages. The results from the simulations were in agreement with the experiments. The use of simulations can provide deeper insights on the behaviour of the molten metals during melting and solidification. However, there is currently no model for

multi-material SLM process. Therefore, a numerical model for multi-material in SLM is developed in this work.

Firstly, discrete element method (DEM) was used to model the powder bed. The powders were released from a height and allowed to fall and scatter randomly, similar to the recoating mechanism in SLM process. A moving laser source was adopted in the model to study the thermal conductivities of single and multi-material powder beds.

Next, a computational fluid dynamics (CFD) approach was used to model the melting and solidification process in the SLM. Information of the powder bed generated using DEM was imported to the CFD solver where a Gaussian heat source is used to melt the powder into a molten pool and the molten metal was allowed to solidify. The dimensions of the molten pool in the model was compared to those measured in experiments in literature to compare the accuracy of the model. The model was used to study the formation of porosities in the SLM process and its relationship with energy density. Two types of porosities were observed. Lack of fusion porosities were formed when low energy density parameters were used. Incomplete melting of the powders resulted in gas trapped between powder particles. Keyhole porosities were observed when high energy density parameters were applied on the powder bed. A deep and unstable keyhole led to the collapse of the keyhole, trapping gas within the molten metal.

Lastly, a multi-material model was built on a modified set of governing equations from the single material model. An additional α phase was added to represent the second metal. The material properties of the mixture of both metals was calculated

using a volume weighted average method. Ti6Al4V powder was deposited on a SS316L baseplate and the laser source scanned across the powder bed. Different values of interfacial tensions between the two materials were used to study their resultant effects on the material mixing during their molten state. A comparison of the melt pool geometries between the simulations and experiment were made to validate the model.

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Journal papers

- (1) Tan, J.L., Tang, C. and Wong, C.H., 2018. A Computational Study on Porosity Evolution in Parts Produced by Selective Laser Melting. *Metallurgical and Materials Transactions A*, 49(8), pp.3663-3673.
- (2) Tan, J.L., Tang, C. and Wong, C.H., 2018. Study and modeling of melt pool evolution in selective laser melting process of SS316L. *MRS Communications*, 8(3), pp.1178-1183.
- (3) Tang, C., Tan, J.L. and Wong, C.H., 2018. A numerical investigation on the physical mechanisms of single track defects in selective laser melting. *International Journal of Heat and Mass Transfer*, 126, pp.957-968.

Conference papers

- (1) Tan, J. L., and Wong, C. H., 2016. Review of Multi-material Additive Manufacturing. *Proceedings of the 2nd International Conference on Progress in Additive Manufacturing (Pro-AM 2016)*, pp.294-299.
- (2) Tan, J. L., Tang, C., and Wong, C. H. 2018. Thermal fluid modelling of selective laser melting. *Proceedings of the 3rd International Conference on Progress in Additive Manufacturing (Pro-AM 2018)*, pp.557-562.
- (3) Tan, J. L., Sorkin, A., and Wong, C.H., 2017. Multi-material modelling for selective laser melting. *9th International Conference on Materials for Advanced Technologies (ICMAT 2017)*, *Procedia engineering*, 216, pp.51-57.

1. Introduction

1.1 Background

Additive manufacturing (AM), or more commonly known as three-dimensional (3D) printing, has seen a surge in interest over the past decade. It is capable of producing parts with complex geometries that traditional manufacturing technology may not be able to. Coupled with the fact that it is economically cost-effective makes it more attractive for industries to incorporate AM into their manufacturing cycle [1]. It can be used for rapid prototyping to test and gather end-user's feedback in a fast and effective manner. Table 1.1 shows examples of the cost-saving effects of using AM. Unlike conventional manufacturing, AM does not require moulds or dies. This avoids the need for manufacturers to purchase them, especially when multiple moulds and dies are used for different parts. With AM being able to manufacture complex shapes, redesign of parts can be carried out. GE Aviation has designed a fuel nozzle that can be printed as a single piece that previously required 20 parts welded together [2]. The ability for AM to print on demand allows companies to reduce the need for spare parts. They only require to store the raw materials such as filaments or powders which take up less inventory space [3].

Table 1.1 Radical reductions in the consumption of non-value adding resources [1]

Example	First order effect	Second order effect
No need for mould/dies	Less material consumption	Lower start-up costs

Fewer parts to join	Less joining equipment	Less capital tied up in infrastructure
Fewer parts to assemble	Less labour and less assembly equipment	No need to off-shore production to low labour cost markets
No spare parts to stock	Less storage space	Reduce factory and warehousing size

AM, the process of building a 3D object by adding layer after layer of raw material, was developed in the 1980s [4]. American Society for Testing and Materials (ASTM) defined AM as a process of joining materials to fabricate parts using 3D model files in a layer by layer method [5]. Stereolithography (SLA), the first approach used in AM, uses ultraviolet (UV) light to cure the surface of a photopolymer vat layer-wise. It takes a computer-aided design (CAD) sketch, slices it into the desired layer thickness and the machine then prints it layer by layer to construct the object. Figure 1.1 shows the process cycle of prototyping involving AM. The first step in product development is to conceptualize the product in terms of how it will look and function. Next, it will be designed using CAD software to form a solid model. In complex geometries, it is difficult to spot errors in the CAD model. Hence, detection of errors and correction can be carried out using computer-aided engineering (CAE) software such as MAGICS. Once the errors are rectified, the file can be converted to STL (Standard Tessellation Language or Stereolithography) files to be printed. The printed part will undergo tests to determine if it meets the design criteria. If further

modifications are required, the cycle will begin from the conceptualization phase. The use of AM shortens duration from design to the testing and evaluation phase.

Figure 1.1 Process cycle of AM [6]

Some benefits of AM are listed below:

1. AM gives more design freedom than conventional manufacturing methods. AM is able to produce complex geometries simply by using CAD to generate the drawing of the model [7]. In traditional manufacturing, designers have to consider the limitations while developing their designs. Now, such limitations are greatly reduced.
2. AM accelerates production cycles. Companies are able to produce prototypes in a shorter time to send for testing and make improvements to their products [8]. By reducing the time to market, companies can ensure their products remain competitive in the market [9].
3. Since AM uses only materials it requires, it enables material wastage to be reduced, unlike conventional manufacturing which subtracts or removes the materials which are not required.
4. AM gives manufacturers the ease of modification of their parts. They only need to make changes to the original CAD file to produce another part. This allows manufacturers to make any improvements in their designs without having to make many changes in the production process.
5. Assembling of parts can be avoided since assembled parts can be printed directly using AM technology. For example, GE Aviation has 3D printed a fuel nozzle that would require 20 pieces to be joined using conventional manufacturing [2].

The applications of AM are not restricted to a specific field. It can be used in the medical industry, where doctors can scan and 3D print a patient's body part for analysing and/or practising before having the actual operation [10]. This will

minimise errors during the procedure. In the aerospace and automotive industries, AM is able to produce functional components to be used in real-life applications. General Electric, an aviation leader in jet engines, has turned to AM technology for its manufacturing operations [11].

AM consists of seven categories based on their processes as shown in Figure 1.2. The material extrusion process involves extrusion of material through a nozzle onto a platform. Fused deposition method (FDM) is a well-known process using material extrusion. It uses a filament that will be heated to its melting point when it passes through the nozzle. The molten filament will be deposited onto the platform where it will solidify. With its low cost of production, FDM printers have become affordable when compared to other AM printers [12]. It mainly uses polymers filaments due to their low melting points.

For material jetting, it operates in a similar manner to a 2D printer. The nozzle or printhead will deposit photopolymers on the platform before being cured by UV light. The deposition of photopolymers can be continuous for polyjet technology (PJT) or drop on demand (DoD). DoD approach is typically used for viscous materials [13].

In binder jetting, a binder is jetted onto the powder bed to bind the powder together. This process is relatively faster than other AM techniques and can process metal and ceramic powders. However, due to the presence of the binders, the structural integrity of the parts is affected.

Similar to binder jetting, Selective laser sintering (SLS), electron beam melting (EBM) and SLM use powder bed as a foundation to build parts. However, unlike binder jetting, these three processes require the powder on the powder bed to be

melted and fused instead of using a binder. Both SLS and SLM use laser beams to selectively melt the powder on the powder bed in an inert gas environment. For SLS, the powder is heated to just below its melting point (sintering), while in SLM, the powder is heated to above its melting point to allow the molten material to fuse and solidify. In EBM, an electron beam is used to melt the powder. A tungsten filament is heated in a vacuum environment to generate electrons [14]. Electromagnets accelerate these electrons and direct them at high speed towards the powder bed which will heat the powder. Since EBM relies on electrons to interact with the powder, the powder has to be electrically conductive.

The direct energy deposition (DED) method is defined as a process where a heat source is used to melt materials as they are being deposited. It consists of a nozzle ejecting powder or wire [15]. The laser beam melts the top layer of the part, creating a molten pool. The material is fed into the molten pool which then solidified [16, 17].

Sheet lamination is an AM technique that joins sheets of materials layer by layer. It includes ultrasonic additive manufacturing (UAM) and laminated object manufacturing (LOM). In UAM, sheets of materials are joined using ultrasonic welding. Computer numerical controlled (CNC) milling is used to create intricate internal structures which conventional manufacturing is unable to replicate [18]. LOM uses adhesive to join sheets of materials [19]. Sheet lamination processes give a faster production time since the cross-sections of the sheets do not have to be scanned by laser or cured by UV light.

Lastly, vat polymerization technique uses a vat containing photopolymer resin [20]. A platform is lowered into the resin to pre-defined layer thickness. A light source will

scan across the cross-section of the platform, curing the liquid resin. SLA and digital light processing (DLP) are the two vat polymerization techniques. In SLA, a UV light is used to cure the resin while in DLP, a digital light projection screen is used [21].

Figure 1.2 Seven categories of AM processes

1.1.1 Overview of SLM

Figure 1.3 shows the interior of a typical SLM machine. In SLM, the powder is supplied from the feed container. Firstly, the powder scraper or recoater will sweep the powder across the build platform, depositing powder with a constant layer thickness between the base plate and the blade of the scraper. The laser source will be guided by the scanner or galvanometric mirrors to different areas of the powder bed. There are two scanner mirrors, each controlling the x -axis or y -axis direction of the laser beam. Next, the laser beam will pass through an f -theta (f - θ) lens. The laser beam consists of many parallel beams. The function of the f - θ lens helps to converge these individual parallel beams onto a specific area known as the laser spot size [22]. Another function of the lens is to ensure that regardless of which area of the powder

bed the laser beam is directed to, the laser spot size and focal length will remain constant to deliver a consistent laser power across the powder bed. When the laser beam scans across the powder bed, the powder will be heated to beyond its melting point and form a melt pool. The melt pool depth will have to be reasonably greater than the layer thickness. This allows the top layer to fuse with the previous layers to avoid delamination of the parts. After the laser has completed scanning the powder bed, the build platform will be lowered according to the layer thickness. The powder scraper or recoater will then deposit a fresh layer of powder and the entire process will repeat until the part is completed. [23]

Figure 1.3 Interior of a typical SLM machine [23]

SLM has the capability to process many materials such as iron (Fe) based and aluminium (Al) based alloys achieving densities of over 99% [24]. By controlling the laser scanning strategies, the properties of the parts can be altered to suit the purpose of their functions [25]. In general, parts produced by SLM exhibit better fracture and impact toughness, and higher hardness compared to conventional manufacturing due to grain refinement strengthening [26]. They can also be heat-treated to attain desired properties [27]. Tables 1.2 to 1.4 shows the comparisons of SLM processed commercially pure titanium (CP-Ti) with other manufacturing methods [28]. Table 1.2 shows the Vickers hardness of the parts produced by SLM, casting and cold working. The SLM part shows a 24% improvement in hardness when compared to casting and is close to the hardness of the cold worked part. Table 1.3 shows the ultimate compressive strength (σ_{UCS}) and maximum strain (ϵ_{max}) between SLM and equal channel angular pressing (ECAP) [29]. Coarse-grain and ultrafine-grain parts were produced using ECAP. The σ_{UCS} of the selectively laser melted part is noticeably better than that of the ECAP part. Its ϵ_{max} is greater than the ultrafine-grain part but slightly lower than the coarse-grain part. Without SLM, users have to compromise on material properties by choosing either coarse-grain with higher ϵ_{max} but lower σ_{UCS} or ultrafine-grain with lower ϵ_{max} but higher σ_{UCS} . With SLM, the advantage from the higher σ_{UCS} can offset its slightly lower ϵ_{max} , improving the material properties of CP-Ti. Table 1.4 shows the yield strength ($\sigma_{0.2}$), ultimate tensile strength (σ_{UTS}) and fracture strain (ϵ_f) of parts produced by SLM and conventional manufacturing methods such as sheet forming and machining. It is

distinct that manufacturing CP-Ti using SLM produced results close to or better than conventional methods.

Table 1.2 Hardness properties of CP-Ti processed by different technologies [28]

Methods	Vickers hardness (Hv)
SLM	261
Casting	210
55% Cold Worked	268

Table 1.3 Compressive properties of CP-Ti processed by different technologies [28]

Methods	σ_{UCS} (MPa)	ε_{max} (%)
SLM	1136 $\pm$ 15	51 $\pm$ 3.5
Coarse-grained (CG-Ti)	820	60
Ultrafine-grained (UFG-Ti)	900	35

Table 1.4 Mechanical properties of CP-Ti processed by different technologies [28]

Methods	$\sigma_{0.2}$ (MPa)	σ_{UTS} (MPa)	ε_f (%)
SLM	555 $\pm$ 3	757 $\pm$ 12.5	19.5 $\pm$ 1.8
Sheet forming	280	345	20
Full annealed	432	561	14.7

1.1.2 Multi-material systems in AM

To further increase the competitiveness of AM, multi-material systems are being developed. Stratasys, a manufacturer of 3D printers, has been able to incorporate multiple materials printing capability into their Polyjet printers. Their printers are able to eject different materials from the two or more jetting heads, usually one material for the main part and the other for the support structure. The materials used are photopolymers which are cured almost instantly by UV light. The support materials are water-soluble to allow for easy removal. Figure 1.4 shows a part made with different materials. The orange part is printed with the main materials while the white part is printed with soluble support materials.

Figure 1.4 Stratasys's multiple material printing using Polyjet technology: (a) before support removal and (b) after support removal [30]

In recent times, there have been extensive researches conducted to allow for multiple materials processing using AM. Table 1.5 shows the different AM techniques and their current progress in multiple material printing. There are two broad categories of multi-material techniques. In vat polymerization, powder bed fusion and sheet lamination, the multi-material process is limited to its deposition method. Only one

material is allowed on each layer for these processes as shown in Figure 1.5(a). To change material during the printing, a layer of different material will have to be deposited and built on the previous material. For processes involving the use of nozzles as a form of delivery mechanism such as material extrusion, binder jetting, direct energy deposition and material jetting, different materials can be deposited within the same layer as shown in Figure 1.5(b). This allows the user to have greater control over the material properties within the build part.

Table 1.5 AM and multi-material AM (MMAM) [31]

Process	Description	Typical AM techniques	Current MMAM techniques	Materials
Photopolymer vat	Liquid photopolymer is selectively cured using a light source	SLA, 2 photon polymerization	SLA	Photo-curable polymers
Material extrusion	Material is selectively dispensed through a nozzle or extruder	FDM, robocasting, bio-plotting	FDM	Polymers, ceramics, metals
Powder bed fusion	Thermal energy selectively fuses regions of powder bed	Selective laser sintering (SLS), SLM, EBM,	SLS	Polymers, metals, ceramics

		Selective mask sintering		
Direct energy deposition	Focused thermal energy melts materials as deposited	Laser engineering net shaping (LENS), Direct metal deposition (DMD)	LENS, DMD	Metals, ceramics
Sheet lamination	Material sheets are bonded together and selectively cut in each layer to create a desired 3D object	Laminated object material (LOM), UAM	LOM, UAM	Metals, ceramics, polymers
Material Jetting	Droplets of build material are selectively deposited layer by layer	DoD, PJT	DoD, PJT	Polymers, metals, ceramics
Binder jetting	Liquid bonding ink is selectively spread to join solid powder material	3DP	3DP	Polymers, metals, ceramics

Figure 1.5 Types of multi-material printing: (a) materials variations restricted to along the build direction and (b) materials variations in any directions

Most polymer AM processes such as SLA and FDM are easily modifiable to suit MMAM. In SLA, a rotating vat carousel system is used to change the resin for the build [32]. In Figure 1.6, there are two vats containing resins of different materials and a vat containing the cleaning solution. Firstly, the platform will be submerged in the vat for material A and the UV light will cure the resin. To switch to material B, the platform will be removed from the vat containing material A and submerged in the vat with a cleaning solution. This is to remove excess material A resins to prevent contamination. The platform will be submerged in the vat containing material B and the UV light will cure the resin of material B.

Figure 1.6 Multi-material stereolithography machine [32]

In an FDM machine, it can have two or more extrusion tips to deposit build materials and support material. To build a part, a thermoplastic filament is heated to its melting point at the nozzle and extruded to the platform [4]. With additional extrusion tips, different materials can be incorporated into the build part [33]. Figure 1.7 shows two FDM machines combined and used a sliding platform to switch between them. FDM1 contains filaments of material A and B, and FDM2 contains filaments of material C and D. When printing material A and B, the build platform will be moved to the building area of FDM1. To change to material C and D, the pneumatic slide will move the build platform to the build area of FDM2.

Figure 1.7 Schematic of multiple material FDM machine [33]

However, due to the recoating mechanism used in powder bed processes such as SLM and SLS, multiple material process proved to be a challenge. Current recoating mechanism covers the layer with single powder material. Therefore, to have another powder on the same layer will require modification to the recoating system.

1.2 Objectives and scope

The objectives of this research consist of the following:

1. To develop a model representing a powder deposition process.
2. To simulate the melting of a single track of a single material and validate the results with experimental data.
3. To simulate the melting of multi-material in SLM process by building on the single material model.

Firstly, the modelling of the SLM can be divided into two processes. The first process is the powder formation and deposition on the substrate. In this work, DEM was used to model the powder particles. The powder was released from a predefined height onto a substrate to allow the powder particles to be scattered randomly. A moving heat source was introduced to study the temperature evolution across the powder bed.

The powder in DEM remained spherical despite the phase change from solid to liquid state, therefore, the powder's properties were imported to a computational fluid dynamics (CFD) model. A single material model was developed to simulate the melting and solidification process of SLM. A single track was scanned and the results from the simulation were compared to experiments to validate the accuracy of the model. The material SS316L was chosen due to the availability of its experimental results from the literature. A study on the porosity formation of a single track was conducted to explain the different types of porosities found in SLM parts.

Next, a multi-material model was developed to study the melt pool. An additional phase, α , was included in the model to represent the additional material. To validate the model, an experiment was conducted by printing Ti6Al4V powder on a SS316L substrate. Cross-sections of the melt pool geometries of the simulations and experiments were compared. Next, studies were carried out on the surface tension between the two materials to observe its impact on the melt pool's formation during the SLM process.

1.3 Organisation of report

In Chapter 1, introduction of AM is given. SLM process is described, and the properties of the printed parts are compared to those traditionally manufactured. Multiple material processing in AM are listed and how some of those techniques are able to accommodate MMAM technology. Outlines of the objectives and scopes are laid out.

Chapter 2 presents the literature survey on AM, primarily focusing on SLM. Previous works on simulation on laser melting process will be presented and discussed. Models using DEM, CFD and lattice Boltzmann method (LBM), which are the common methods used to model the SLM process, will be reviewed.

Chapter 3 will present results on the powder deposition process using DEM. A model consisting of different material powders was heated by a moving heat source along the interface to observe the heat transfer between the powders via conduction.

Chapter 4 will discuss on the melting and solidification of SS316L powder bed using CFD to model the SLM process. The powder characteristics were imported from the DEM model and a substrate was included in the model. A moving Gaussian-based heat source was used to simulate the laser beam of the SLM. A porosity study was conducted to compare the simulation results with experimental results to validate the model.

Chapter 5 investigates multi-material modelling by modifying the single material solver. An additional phase, α , was introduced to the volume of fluid (VOF) equation to represent the addition of a new material in the model. In this chapter, Ti6Al4 powder was modelled on a SS316L substrate. A moving heat source melts

the powder and the substrate to form a single track. Experiments were conducted with similar powder and substrate materials to validate the simulation results. Cross-sections of the melt pool were compared to determine the accuracy of the model. Different interfacial tensions between Ti6Al4 and SS316L were modelled to compare the effects of interfacial tension on the mixing within the melt pool.

Finally, Chapter 6 will present the conclusions of the thesis and the possible future works from current progress.

2. Literature Review

2.1 Introduction

This chapter focuses on literature reviews on experiments and simulations using different welding techniques and AM. Similar to SLM, welding processes use a heat source to melt materials. Hence, previous work on welding can provide insights on the melting and solidification process which also takes place in the SLM process. There are works on the joining of dissimilar metals in welding which can be applied to multi-material SLM process. However, welding primary usage is for joining of parts instead of building layer-by-layer. Simulation methodology and results using different modelling techniques on the laser melting process will be discussed. DEM was adopted to deal with the interactions between powder particles and to model the powder deposition process, while CFD was used to solve for the fluid flow during the melting and solidification of the powder particles.

2.2 Welding

In current society, there is an increasing demand for the use of two or more metals in a part. This allows for adoptions of each metal's specific property to suit the functionality of the component. Welding is a conventional manufacturing method used to form metal to metal joints [34]. Forge welding is the oldest technique of welding where two pieces of metals are heated, hammered and pressed together to allow for joining at the surface.

An alternative welding process is fusion welding. It requires for the two metals to be melted and fused. This process requires intense heat to be supplied to the joint [35]. Arc welding and laser beam welding are examples of fusion welding. Figure 2.1 illustrates a fusion weld. A liquid weld pool is formed when the metals are heated to their melting points and they will start to fuse together upon solidification. The fusion zone is where the metals undergo melting and solidification. The heat-affected zone will experience huge thermal exposure and solid-state transformation, but no melting occurs.

Figure 2.1 Schematic of fusion welding [36]

2.2.1 Laser beam welding

Laser beam welding (LBW) uses a keyhole fusion welding technique with high power density laser beam focusing on a fine spot [37]. At the surface, the focused beam will generate enough thermal energy to melt the metals, slowly progressing through the joint. The concentrated thermal energy produces melting and yields a narrow heat-affected zone. This helps to retain the metals' mechanical properties [38].

The weldability of dissimilar metals can be determined by their crystal structure, atomic diameter and compositional solubility in both solid and liquid states [39]. Certain metals such as copper and aluminium are difficult to melt due to their high reflectivity and thermal conductivity. Formation of intermetallic phases also poses a problem for joining dissimilar metals [40]. Intermetallic phases tend to be brittle and promote cracks which is detrimental to the mechanical property of the part [41].

A study of dissimilar joints using laser welding was conducted by Mai et al [39]. Dissimilar joints comprising Kovar-tool steel, copper-tool steel and copper-aluminium were experimented. Results at the interface regions are shown in Figures 2.2 to 2.4.

Figure 2.2 Welded sample of Kovar and tool steel: (a) top view with 1.3 mm seam, (b) cross-section at 50× magnification [39]

Figure 2.3 Welded sample of copper and tool steel: top view with 1.3 mm seam, (b) cross-section at 50×magnification [39]

Figure 2.4 Welded sample of copper and Al 4047 aluminium alloy: top view, (b) cross-section at 20×magnification [39]

Figure 2.2(b) shows the presence of convection current in the weld pool and pores found in the middle of the current. This is due to the rapid cooling which trapped the pores. In Figure 2.3(b), the copper did not bond well with the tool steel at the interface. Since copper has a high conductivity, it will cool down faster than the tool steel reducing the amount of mixing. The fusion zone in Figure 2.4(b) shows the copper and aluminium alloy interface with more of the latter, represented by the dark region, flowed towards the interface. Using energy dispersive x-ray spectroscopy

(EDX), Mai et al. observed the fusion zone consisted of 48% Al and 27% Cu. The high reflectivity of copper results in less of it being melted.

To resolve the issues of high reflectivity in copper, a study was performed on copper and steel yielding positive results. Figure 2.5 shows the interface between copper and the weld region. Complete metallurgical bond was achieved by using slope butt joint as shown in Figure 2.6, while focusing the laser beam more towards the steel [42]. Figure 2.6(a) shows the laser beam melting the steel plate to generate a weld pool. Heat from the weld pool will be dissipated to the surrounding steel and copper plates. With sufficient heat energy, the copper plate will begin to melt as seen in Figure 2.6(b). A thin layer of fusion zone is formed between the steel and copper. The top surface of the weld will have a wider fusion zone compared to the bottom shown in Figure 2.6(c). This is due to the laser generating more heat at the top surface which resulted in more copper being melted due to heat transferred from the weld pool. It was concluded that limiting the amount of copper in the molten steel can reduce the number of defects found in the joint.

Figure 2.5 Interface between copper and steel using LBW [42]

Figure 2.6 (a) Formation of melt pool on steel plate, (b) melt pool extends towards copper plate and (c) intermixing between steel and copper [42]

2.2.2 Electron beam welding

Electron beam welding (EBW) is another method of fusion welding. Unlike LBW, EBW uses electrons and operates in a vacuum environment [43]. The weldability of different metal combinations is shown in Table 2.1. The weldability chart determines the compatibility of weld between the metals. From the table, nickel (Ni) and Cu can be fully soluble in welding resulting in a strong weld joint. Welding Al and titanium (Ti) will lead to formation of intermetallic compounds as observed by Jiangwei et al. [44]. Ghosh et al. studied that the presence of intermetallic compounds will lower the strength at the joints [45].

Table 2.1 Weldability of dissimilar metal combinations using EBW [46]

Al	2																
Au	1	5															
Be	5	2	5														
Co	3	5	2	5													
Cu	2	2	1	5	2												
Fe	3	5	2	5	2	2											
Mg	5	2	5	5	5	5	3										
Mo	3	5	2	5	5	3	2	3									
Nb	4	5	4	5	5	2	5	4	1								
Ni	2	5	1	5	1	1	2	5	5	5							
Pt	2	5	1	5	1	1	1	5	2	5	1						
Re	3	4	4	5	1	3	5	4	5	5	3	2					
Sn	2	2	5	3	5	2	5	5	3	5	5	5	3				
Ta	5	5	4	5	5	3	5	4	1	1	5	5	5	5			
Ti	2	5	5	5	5	5	5	3	1	1	5	5	5	5	1		
W	3	5	4	5	5	3	5	3	1	1	5	1	5	3	1	2	
Zr	5	5	5	5	5	5	5	3	5	1	5	5	5	5	2	1	5
	Ag	Al	Au	Be	Co	Cu	Fe	Mg	Mo	Nb	Ni	Pt	Re	Sn	Ta	Ti	W

1. Very desirable (solid solubility in all combinations), 2. Probably acceptable (complex structures may exist), 3. Use with caution (insufficient data for proper evaluation), 4. Use with extreme caution (no data available), 5. Undesirable combinations (intermediate compounds may be formed)

Studies have been conducted to weld dissimilar metals using EBW with high energy density. The small beam size in EBW allows better control over the dilution of the weld [47]. An investigation on copper-stainless steel microstructures was conducted by Magnabosco et al. [48]. Figure 2.7 shows the interfaces between the weld zone and the two metals. No cracks or porosity was observed in the metallographic inspections for the first joint using a single pass weld to join a 33 mm Cu plate with a 29 mm SS304L plate. However, there were presence of cracks in the second and third joints when a double pass welding technique was used to join thicker plates, as shown in Figures 2.8 and 2.9. Copper diffusion led to the embrittlement of the

austenitic grain boundaries and promote cracks due to solidification shrinkage. This can be substantiated by the presence of copper traces found in the cracks and was also reported by Mai et al. in laser welding [39].

Figure 2.7 (a) Weld interfaces of copper-weld region and (b) weld region-stainless steel for first joint [48]

Figure 2.8 Cracks at interface of weld region and stainless steel [48]

Figure 2.9 (a) Weld interfaces of copper-weld region, and (b) weld region-stainless steel for third joint [48]

While Table 2.1 shows Cu and Fe have good weldability, Magnabosco et al. demonstrated that cracks and porosities defects can be formed when wrong process parameters were used. This demonstrates the importance of using the right process parameters for the joining dissimilar metals. Similar to EBW, AM processes that provides high energy density sources such as SLM and EBM have the potential to manufacture parts with dissimilar metals. Observations from EBW, such as copper diffusion leading to embrittlement, can be used to avoid defects in AM processes.

2.3 Selective laser melting

Producing multi-materials parts using SLM process is a challenging task. Current SLM machines are limited to single material due to the powder deposition process. However, modifications can be made to the recoating systems of machines to allow the deposition of different materials along the build direction as shown in Figure 2.10 [49]. Regenfuss et al. made use of two recoaters to hold copper and silver powders individually in Figure 2.10(a). To deposit silver powder, the recoater with the silver powder will sweep across the build platform to spread a layer of silver powder. The

laser will scan the powder before the platform lowers. To switch to copper powder, the recoater containing the copper powder will sweep across the platform to deposit copper powder. By the recoaters deposition mechanism, a part can have multiple materials varying along its build direction as shown in Figure 2.10(b).

Figure 2.10 (a) Multiple recoating mechanism and (b) laser micro sintered part with different materials along its build direction [49]

In the works of Liu et al. [50] and Sing et al. [51], the SLM250HL from SLM Solutions Group AG was used to print a multi-material part using copper alloy C18400 and SS316L powders. The machine has a forward and backward recoating mechanism. Users are able to select different recoating configurations: forward recoating, backward recoating or both. Powder will be deposited when the recoater moves forward or backward. Figure 2.11(a) shows the chamber of SLM250HL and Figure 2.11(b) shows the top view of the recoater. The divider in the recoater helps to feed the powder to two separate rollers in the recoater. The rollers have grooves to carry the powder from the recoater to the platform when they rotate. Figure 2.12 shows a schematic of the powder deposition process in the machine. Each roller was programmed to rotate for each recoating direction. Sing et al. modified the recoater by compartmentalising

the recoater to two compartments – one for each material. Therefore, when the machine was set to forward recoating configuration, only SS316L powder was deposited. Switching to backward recoating configuration will allow the copper powder to be deposited. Figure 2.13 shows the multi-material parts printed using this approach.

Figure 2.11 (a) Interior build chamber of SLM250HL and (b) top view of recoating showing the divider feeding the powder to the rollers

Figure 2.12 Schematic of multi-material deposition in SLM250HL showing the delivery of powders in a two-way recoating system [52]

Figure 2.13 Multi-material parts printed using SLM250HL using C18400 and SS316L [52]

Figure 2.14 (a) Powder bed with multiple materials in SLM250HL, (b) multi-material part

In Figure 2.14, SS316L and K220 copper alloy powders were mixed within the same layer as well as between layers leading to contamination of the powders. One of the problems faced conducting these experiments was the recyclability of the powders. While Chivel [53] has suggested using powders of varying diameters for each material, it would not eliminate the contamination completely. However, the diameters of the powders may change during the SLM process due to spattering and it will be impossible to track change in diameters of the powders.

The phenomena of spattering in SLM may result in the diameters of the spattered powder being larger than the fresh powder. Spattered powders are found on the powder bed as observed by Anwar et al. [54, 55]. Figure 2.15 shows the size distribution of the fresh powders and spattered powder 1 measured by Liu et al. which are labelled as powder 1, powder 2 and spatter respectively [56]. When the laser scans powder 1, the powder will be melted into its molten state. The recoil pressure may eject some molten powder 1 from the melt pool. When the ejected powder collides with each other, they will fuse and form a larger particle [57]. Therefore, despite

powder 2 being larger in diameter, the spatter of the smaller powder 1 falls under the size distribution range of powder 2 as shown in Figure. 2.15.

Figure 2.15 Diameter distributions of powder 1, powder 2 and spatter of powder 1

For single material, experiments can be conducted for parametric analysis and the unused powder in the powder bed can be recycled for future use. However, the powders in the multi-material powder bed shown in Figure 2.14 cannot be separated. To overcome the issue of material wastages, computational simulations can be carried out to observe the interactions between materials during the laser melting process. Studies using computational methods have been used for single materials and the results were validated with experimental results [58, 59, 60]. Wu et al. found the simulation result of the melt pool geometry was comparable to that of the experiment.

This shows simulations are able to provide a good representation of the results obtained with experiments.

2.4 Discrete element method

DEM is a numerical method to simulate the movement of a granular material by solving Newton's second law [61]. When two or more particles are in direct contact, the linear and rotational motion can be expressed by the summation of the forces and moments with neighbouring particle expressed as [61, 62, 63].

$$m_i \frac{d^2 x_i}{dt^2} = m_i \cdot g + \sum_{j=1}^N F_{ij} \quad (2.1)$$

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^N (r_i \times f_{ij}) \quad (2.2)$$

where m_i is the mass of particle i , x_i is the position of particle i , g is the gravitational constant, N is the number of neighbouring particle in contact, F_{ij} is the normal contact force on particle i by particle j , f_{ij} is the frictional force acting on particle i by particle j , ω_i is the angular velocity of particle i , and r_i is the radius of particle i .

Zohdi studied the effects of laser on particulate matters with different thermal conductivities [64]. In his model, discrete ray tracing was used. The 1000 rays were traced over 20 pulses. To determine the phase transformation of the powder, comparisons between the temperature of the powder with the melting and vapourizing points were conducted. However, no physical phase change can be observed in the

model. Figure 2.16 shows the laser rays heating the powder bed and the change in temperatures of the powder. The orange arrows represent individual ray of the laser beam. Zohdi employed ray tracing with Fresnel reflection to determine the absorption of laser ray by the particle. Figure 2.16(a) shows the rays before hitting the powder bed and Figure 2.16(b) shows the reflected path of the rays after hitting the powder. The top powder particles absorbed energy from the rays and were heated up. These particles will conduct heat to the neighbouring particles.

Figure 2.16 (a) Laser rays before hitting the powder bed, (b) laser rays reflected after hitting the powder bed [64]

Further work was done by Ganeriwala with a moving heat source [65]. In this model, the laser scanned in a zig-zag pattern as seen in Figure 2.17. The laser intensity was assumed to be constant within the laser spot size instead of the Gaussian distribution observed in actual experiment. The simulation model was assumed to be adiabatic, meaning there is no heat transfer through the simulation boundaries. A correlation

was established between the particle size and its temperature. Smaller particles show a higher average temperature than large particles and can be explained by

$$Q = cm\Delta T \quad (2.3)$$

where Q is the heat input by the laser, c is the specific heat, m is the mass and ΔT is the change in temperature. With similar heat input and specific heat, smaller powder having smaller mass will lead to greater change in temperature.

Figure 2.17 (a) First track scanned in positive x direction , (b) second track scanned in negative x direction, (c) third track scanned in positive x direction and (d) fourth track scanned in negative x direction [65]

A study was done by Ganeriwala et al. [66] using DEM. The powders were allowed to be deposited onto the substrate with the help of gravity as shown in Figure 2.18. A laser beam, following a Gaussian distribution, was passed over the layer and a temperature gradient can be observed in Figure 2.19. The laser intensity is assumed to decrease exponentially with depth z and is expressed as

$$I = I_0 e^{-\beta z} \cdot e^{(-2r^2/d)} \quad (2.4)$$

where I_0 is the peak intensity, d is the beam spot size measured to where intensity dropped to $1/e^2$, β is the optical extinction coefficient, and r is the radial distance from beam centre. In this model, heat transfer due to conduction, convection and radiation was considered. The material properties of the powder were altered based on their temperatures to account for the differences of the properties during phase change.

Figure 2.18 Deposition of a layer of powder [66]

Figure 2.19 Temperature gradient when laser passed over powder layer [66]

Ganeriwala et al. compared their simulation results to experiment conducted by Khairallah et al. [58]. The melt pool's depth, width and height were listed in Table 2.2. They attributed the main source of error due to the lack of Marangoni convection and surface tension present in fluid flow.

Table 2.2 Comparison between simulation and experimental results [66]

	Simulation	Experiment	Deviation (%)
Height (μm)	30	26	15.4
Width (μm)	85	75	13.3
Depth (μm)	20	30	33.3

2.5 Computational fluid dynamics

The foundations of CFD are based on three principles [67, 68]:

- 1) conservation of mass (continuity equation)
- 2) conservation of momentum (Newton's second law)
- 3) conservation of energy (first law of thermodynamics)

The continuity equation can be represented by [69]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 \quad (2.5)$$

where ρ is the density of fluid, t is time and $\vec{V}$ is the velocity vector.

The conservation of momentum which can be represented by the Navier-Stokes equation in x , y and z components respectively is computed as.

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u \vec{V}) = -\frac{\partial P}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x \quad (2.6)$$

$$\frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v \vec{V}) = -\frac{\partial P}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + \rho f_y \quad (2.7)$$

$$\frac{\partial(\rho w)}{\partial t} + \nabla \cdot (\rho w \vec{V}) = -\frac{\partial P}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z \quad (2.8)$$

where u , v and w are the velocities in the x , y and z components respectively, P is the pressure, τ is the viscous stress and f is the body forces.

The conservation of energy is given by

$$\begin{aligned}
& \frac{\partial}{\partial t} \left[\rho \left(e + \frac{u^2 + v^2 + w^2}{2} \right) \right] + \nabla \cdot \left[\rho \left(e + \frac{u^2 + v^2 + w^2}{2} \right) \vec{V} \right] \\
&= \rho \dot{q} + \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) \\
&\quad - \frac{\partial(uP)}{\partial x} - \frac{\partial(vP)}{\partial y} - \frac{\partial(wP)}{\partial z} + \frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} \\
&\quad + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(w\tau_{zz})}{\partial z} \\
&\quad + \rho \vec{f} \cdot \vec{V}
\end{aligned} \tag{2.9}$$

where k is thermal conductivity, $\dot{q}$ is volumetric heat transfer rate per unit mass and T is temperature.

2.5.1 Algorithms for pressure-velocity coupling

In most scenarios, the velocity and pressure fields are unknown. For a compressible flow, there is an additional equation of state relating pressure, velocity and temperature [70]. However, for incompressible flow, the density is constant and is unrelated to pressure. An iterative method, widely known as SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm, was introduced by Patankar and Spalding [71, 72]. Figure 2.20 shows a flowchart of the SIMPLE algorithm [73]. The initial values of pressure field are estimated and used to solve for the discretised momentum equations to give the velocities. Next, solving the pressure correction equation will yield a corrected pressure. The corrected pressure field is used to solve for the corrected velocities. With the corrected pressure and velocities, the other quantities can be solved using the transport equations. If the solutions do not

converge, the corrected values will be replaced as the estimated values and the iterations will continue.

Figure 2.20 SIMPLE algorithm flowchart [73]

Another algorithm is the Pressure Implicit with Splitting of Operators (PISO) by Issa [74]. The PISO algorithm involves addition correction step from the SIMPLE algorithm shown in Figure 2.21. SIMPLE is useful for correcting velocities but it is less efficient in correcting pressure. The second pressure correction in PISO proved

to be more effective in correcting the pressure field. However, it requires more computational efforts.

Figure 2.21 Flowchart for PISO algorithm [73]

2.5.2 Numerical models for laser welding

Laser welding shares a close resemblance to the SLM process. Both processes use Gaussian laser beams and involve phase change from solid metal to molten metal. Otto et al uses OpenFOAM® (Open Field Operation and Manipulation) to model the laser welding process using PISO scheme [75]. Geiger et al. studied the melt pool dynamics and defects of laser welding using similar model [76]. Pang et al. compared the time taken for the keyhole depth to be stabilize with experiments and found them to have the same magnitude as experiments [77]. Mahrle and Schmidt established similar relationships between the seam width and welding speed from experiments and simulations [78]. Numerical models can be used to predict defects formation during the welding process. Panwisawas et al. used CFD model to predict the porosity formation for different weld plate thickness and the results are consistent with experimental results [79]. These findings show modelling is able to closely predict experimental results and it can be used to simulate results that are difficult to be conducted experimentally.

There are laser welding simulations of dissimilar metals validated with experimental results. Chakraborty modelled copper-nickel dissimilar metal laser welding [80]. He studied the effects of laminar and turbulent models and found out that the distributions of the metals in the turbulent model are consistent with experiments. Métais et al. modelled a full penetrated laser welding on nickel and steel joints [81]. They observed similar hourglass shape and the dimensions of the weld shape are in agreement with experiments. Esfahani et al. performed numerical simulations to predict the dilution and homogeneity of a laser welded joint of carbon steel and stainless steel [82]. They observed that thermal gradient and surface tension have

significant influence over the melt pool geometry. Figure 2.22 shows the experimental weld pools and the simulation weld pools using different specific point energies of 10 J, 17 J and 50 J. For different specific point energies, the simulated weld pool geometry is able to closely predict the shape of the experimental results. For the dissimilar metals models, the top surfaces were assumed to remain flat. They are essentially a two-phase model consisting of only two metals.

Figure 2.22 Experiment weld pool geometry and simulated results for stainless steel (SS) and carbon steel (CS) using specific point energy of (a) 50 J, (b) 17 J and (c) 10 J [82]

2.5.3 Numerical models for SLM

Panwisawas and Qiu et al. have extensively studied the modelling technique of SLM using OpenFOAM® software [83, 84, 85]. Panwisawas studied the effect of layer thickness on the formation of a single track [83]. He concluded that increasing layer

thickness will generate rugged tracks and increase discontinuities of the track. Figure 2.23 shows the formation of porosities on a thick powder bed. The red region represents the metal powder, blue region represents air and green region represents the interface of powder and air. Laser power of 400 W was used with different scanning speeds of 2000 mm/s and 4000 mm/s to simulate different energy densities. Figure 2.23(a) shows spherical pores trapped when sufficient energy density is used to melt the top layer and partially melting the bottom layer when 2000 mm/s scanning speed was used. By reducing the scanning speed to 4000 mm/s, the energy density is halved. Figure 2.23(b) shows elongated pores when the energy density is halved. The top layer was partially melted while the bottom layer was not melted.

Figure 2.23 Solid fraction of powder layer using laser power of 400 W with (a) scanning speed 2000 mm/s and (b) 4000 mm/s [84]

Gürtler et al. modelled a powder bed with a uniform diameter in a face-centred cubic configuration to reduce the complexity of the model [86]. They also assumed the physical material properties are temperature independent to save on computational time. They observed that low power gave rise to porosities in their model due to incomplete fusing of powder with the base plate. Figure 2.24 shows a comparison between the porosities in experiment and their model.

Figure 2.24 Porosities observed in (a) experiment and (b) simulation [86]

Yuan et al. used FLUENT software [87] to study the molten metal flow due to Marangoni effect and temperature distribution during the SLM process [88]. They observed that the Marangoni effect has significant effects on the melt pool's width and depth.

Lawrence Livermore National Laboratory created their solver ALE3D software which uses arbitrary Lagrangian–Eulerian method to solve for multi-physics numerical simulations [89]. Khairallah and Anderson studied the effects of surface tension on the continuity of a single track without considering recoil pressure and Marangoni convection [58]. They concluded that surface tension leads to Plateau-Rayleigh instability of the melt pool, resulting in discontinuous track which can be observed in experiments by Li et al [90]. Khairallah et al. further expand on the model by introducing recoil pressure and Marangoni convection [91]. They observed that recoil pressure creates a keyhole and is responsible for the spatter of material when it overcomes the effect of surface tension. Marangoni convection aids in the cooling of the molten metal and pulls surrounding powder particles into the melt pool, creating a denudation zone. King et al. observed melting of overhangs can arise in discontinuous track in the initial layer [92]. When a second layer of powder is

deposited, the discontinuous track acts as a support for the fresh powder. Hence, continuous tracks can be formed on the subsequent layers with the bottom layer supporting the newly formed track as shown in Figure 2.25.

Figure 2.25 Single track geometries of overhang in multi-layers [92]

2.6 Lattice Boltzmann method

Most CFD software solves for the Navier-Stoke equations as shown in section 2.5. However, the LBM is another branch of CFD which solves for the Boltzmann equation instead of Navier-Stoke equations. LBM treats the fluid as a collection of particles and solves for a simplified kinetic equation based on the distribution function of the particles [93]. Incompressible Navier-Stokes equations can be obtained by solving Boltzmann equation in certain limits [94]. He and Luo

demonstrated the derivation of Navier-Stokes equations from Boltzmann equation using Chapman–Enskog procedure [95].

Körner and Attar modelled the SLM process with LBM in 2D [96, 97, 98, 99]. They adopted the passive scalar approach to determine the temperature field as shown by Shan [100]. They observed that increasing the packing density will give a more defined melt pool shape. They also investigated the influence of process parameters such as scanning speed and laser power on the resultant melt pool track. They found that high laser power and low scanning speed produced continuous track while low laser power and high scanning speed produced small semicircle droplets. However, their model is only able to provide limited insights due to it being 2D.

Bauereiß et al. used similar model to model the defects presence in the powder bed process [101]. Using three different laser powers to scan 20 layers, their simulation results showed the formation of porosities. Their simulation results in Figure 2.26 share similarities with their experiments as seen in Figure 2.27. Laser power of 90 W resulted in extreme porosities while laser power of 180 W showed almost no porosity in both simulations and experiments.

Figure 2.26 Simulations of 20 layers of 50 μm using laser powers of (a) 90 W, (b) 120 W and (c) 180 W [101]

Figure 2.27 Experiment cross-sections for different laser powers of (a) 90 W, (b) 120 W and (c) 180 W [101]

Klassen et al. improved on the model by including recoil pressure induced by evaporation of the material [102]. Their simulations and experiments showed that the

beam width has a strong impact on the mass loss of the material. They also concluded that there is a line energy where the recoil pressure and mass loss are independent on the scanning speed. This allows the scanning speed to be increased without experiencing the negative effects of recoil pressure.

2.7 Summary

Multi-material process in SLM is a challenge due to its complexity in carrying out the experiments. The use of numerical modelling can assist in providing insights on the physical phenomena within the melt pool during the melting and solidification process. There have been numerous studies on laser melting processes simulations that have been validated by experiments. Defects such as porosity and balling can be observed in simulations and experiments using the same processing parameters.

However, there is no existing model for multi-material SLM process. The physical and chemical properties of the materials and their interactions during their molten state can play an important role in defects formation.

3. Discrete Element Method Model

3.1 Introduction

This chapter will discuss on the work using DEM to model the powder bed of the SLM process. The powder diameters in the model follow a Gaussian distribution, similar to the powder used in experiments. To scatter the powder randomly, the powder was set at a predefined height of 700 μm and released. The particles will interact with each other due to the contact forces and allowed time to settle.

A model consisting of a single material powder, SS316L, was heated using a Gaussian heat source to observe the heat transfer through conduction. Subsequently, a powder of different material, Ti6Al4V, was added to the model to simulate a multi-material powder bed.

3.2 Methodology

The open sourced DEM software used is LIGGGHTS® (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations) software [103]. In this software, the particles were modelled as granular system governed by the conservation of momentum in Equations 2.1 and 2.2. It involves a series of process. Firstly, the details of the system are defined. This includes the boundaries of the system, contact model used to model particles interactions, initial conditions, the physical properties of the particles and the timestep. Next, the model will detect for particles collisions. It will solve for the resultant forces acting on each particle and determine the new velocity and acceleration. The displacements of the particles will

be calculated and the particles positions will be updated. The timestep will be increased and the system will detect for collisions. This cycle repeats until the end of the predefined number of timesteps.

3.2.1 Contact models

There are two main contact models in LIGGGHTS® software: linear contact model and Hertz contact model. The linear contact model, also known as Hooke's law, can be expressed as a linear spring system with normal contact force, F , given by

$$F = k\delta \quad (3.1)$$

where k is the spring stiffness and δ is the relative displacement.

Hertz contact model relates the contact force with a non-linear stiffness function, K , which depends on the material properties and shape of contact surfaces [104, 105]. It is given by [106]

$$F = \left(K_n \delta_{n_{ij}} - \gamma_n V_{n_{ij}} \right) + \left(K_t \delta_{t_{ij}} - \gamma_t V_{t_{ij}} \right) \quad (3.2)$$

where i and j are the two particles, K_n is the elastic constant for normal contact, $\delta_{n_{ij}}$ is the normal overlap distance of two particles, K_t is the elastic constant for tangential contact, $\delta_{t_{ij}}$ is tangential displacement vector between two spherical particles which is truncated to satisfy a frictional yield criterion, γ_n is the viscoelastic damping constant for normal contact, γ_t is the viscoelastic damping constant for tangential contact, $V_{n_{ij}}$ is the normal component of the relative velocity of the two

particles and $V_{t_{ij}}$ is the tangential component of the relative velocity of the two particles.

The K_n , K_t , γ_n and γ_t can be calculated using material properties and are expressed as

$$K_n = \frac{4}{3} Y^* \sqrt{R^* \delta_n} \quad (3.3)$$

$$\gamma_n = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} \quad (3.4)$$

$$K_t = 8 G^* \sqrt{R^* \delta_n} \quad (3.5)$$

$$\gamma_t = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m^*} \quad (3.6)$$

$$S_n = 2 Y^* \sqrt{R^* \delta_n} \quad (3.7)$$

$$S_t = 8 G^* \sqrt{R^* \delta_n} \quad (3.8)$$

$$\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}} \quad (3.9)$$

$$\frac{1}{Y^*} = \frac{(1 - \nu_i^2)}{Y_i} + \frac{(1 - \nu_j^2)}{Y_j} \quad (3.10)$$

$$\frac{1}{G^*} = \frac{2(2 - \nu_i)(1 + \nu_i)}{Y_i} + \frac{2(2 - \nu_j)(1 + \nu_j)}{Y_j} \quad (3.11)$$

$$\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j} \quad (3.12)$$

$$\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j} \quad (3.13)$$

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

The advantage of using Hertz contact model is that it considers the geometric and material properties of the contacting surface which is important in contact dynamic response [107]. Hence, Hertz contact model was used in this work to provide a more accurate result of the particles interactions.

3.2.2 Heat transfer

LIGGGHTS® software calculates the heat conduction between particles in contact and updates the temperature using [108]

$$\dot{Q}_{ij} = h_c \Delta T_{ij} \quad (3.14)$$

$$h_c = \frac{4k_i k_j}{k_i + k_j} \sqrt{A_{ij}} \quad (3.15)$$

$$m_p c_p \frac{dT_i}{dt} = \sum \dot{Q}_{ij} + \dot{Q}_{i,source} \quad (3.16)$$

where $\dot{Q}_{ij}$ is the heat transfer between particle i and particle j , h_c is the heat transfer coefficient, ΔT_{ij} is the temperature difference between the particles, k_i is the thermal conductivity of particle i , k_j is the thermal conductivity of particle j , m_p

is the mass of particle, c_p is the specific thermal capacity, A_{ij} is particles contact area and $\dot{Q}_{i,source}$ is the heat generation due to sources.

To model the heat source, a spherical region was defined and the particles within the sphere were assigned a uniform heat source [109]. The centre coordinates of the sphere were set at $x = 100 \text{ } \mu\text{m}$, $y = 200 \text{ } \mu\text{m}$ and the height was set at the top surface of the powder bed. The heat source will travel along the x -axis.

3.2.3 Model set up

In a single material model, the simulation box was set at $1000 \text{ } \mu\text{m} \times 400 \text{ } \mu\text{m} \times 1000 \text{ } \mu\text{m}$. SS316L powder was modelled and the material properties are shown in Table 3.1 [110]. The particle diameters follow a Gaussian distribution with a mean diameter of $27 \text{ } \mu\text{m}$. The particles were released from a height of $700 \text{ } \mu\text{m}$ to scatter randomly. Figure 3.1(a) shows the start of the powder deposition and Figure 3.1(b) shows the end of the deposition process. The particles diameters were represented in colour coding to show the distribution size. Figure 3.1(b) shows the random scattering of particles with different diameters.

Table 3.1 Material properties of SS316L

Physical Properties	SS316L
Density (kg m^{-3})	8000
Thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)	9
Heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$)	462
Young's modulus (GPa)	206
Poisson ratio	0.25
Coefficient of restitution	1.05

Figure 3.1 (a) Start of powder deposition process and (b) end of powder deposition process. The particle sizes are represented by the colour coding

In a multi-material DEM model, SS316L and Ti6Al4V powders were modelled in a $1000\text{ }\mu\text{m} \times 400\text{ }\mu\text{m} \times 1000\text{ }\mu\text{m}$ simulation box. They were released from a height of $700\text{ }\mu\text{m}$. Diameters of both powders follow a Gaussian distribution with mean $27\text{ }\mu\text{m}$. Table 3.2 shows the material properties of Ti6Al4V used [110, 111]. The powder deposition process of each powder was compartmentalized as shown in Figure 3.2(a). An imaginary wall was fixed along $y = 200\text{ }\mu\text{m}$. SS316L powder was released in the region of the box where $0 \leq y < 200\text{ }\mu\text{m}$ and the Ti6Al4V powder was released in the region of the box where $200 \leq y \leq 400\text{ }\mu\text{m}$. Once the powders were deposited, the imaginary wall was removed to allow the powders to mix at the interface as seen in the perspective view in Figure 3.2(b).

Table 3.2 Material properties of Ti6Al4V

Physical Properties	Ti6Al4V
Density (kg m^{-3})	4400
Thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)	21
Heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$)	670
Young's modulus (GPa)	119
Poisson ratio	0.34
Coefficient of restitution	0.8

Figure 3.2 (a) Start of deposition and (b) after deposition process. Yellow powder represents SS316L and blue powder represents Ti6Al4V

3.3 Results and discussions

3.3.1 Single material

A heat source of 300 W with 80 μm diameter was scanned along the x axis at 1.2 m/s. The timestep for the model is 0.125 ns. Figure 3.3 shows the temperature evolution of the powder at different time intervals. At $t = 12.5 \mu\text{s}$, the powder was beginning to heat up from the heat source in Figure 3.3(a). The temperature of the powder did not immediately reach the melting point at 1700 K. The powder was observed to begin melting at $t = 87.5 \mu\text{s}$ seen in Figure 3.3(b). As time progressed, the heat from the powder particles within the heat source started to spread to their neighbours via conduction seen in Figure 3.3(c). The temperature of the melt pool was observed to cool down at a slow rate. In this model, the only mode of heat transfer away from a particle is by the conduction of its neighbouring particles. From Equation 3.15, the conduction is dependent on the contact area of the particles. As the particles have small contact area, this greatly limits the amount of heat being transferred from particle to particle.

Figure 3.3 Temperature evolution of top view and cross-sectional view at $x = 100 \mu\text{m}$ at: (a) time = $12.5 \mu\text{s}$, (b) time = $87.5 \mu\text{s}$ and (c) time = $887.5 \mu\text{s}$

The melt pool was observed to have a depth of $117 \mu\text{m}$ and width of $147 \mu\text{m}$ in Figure 3.4. When compared to experimental results by Kamath et al. [110], their measured depth was $114 \mu\text{m}$ and width was $111 \mu\text{m}$. This huge difference in width can be attributed to the lack of heat loss in the model. This model did not account for heat loss through convection, phase change and evaporation which play a major part in heat removal from the melt pool [58].

Figure 3.4 Cross-section of melt pool geometry

3.3.2 Multi-material

In the multi-material powder bed, a heat source of 300 W with scanning speed of 1.2 m/s was scanned along the interface of the powders. Figure 3.5 shows the cross-section of the temperature of the powders at different time intervals. Figure 3.5(a) shows the temperatures of the powders when the laser begins to heat up the powders. The temperatures of the powders of each material was observed to be relatively symmetrical along the interface. This is because the volumetric heat capacities of both materials differ by approximately 20% shown in Table 3.3.

At $t = 887.5 \mu\text{s}$, the temperature profile of the powders had an observable difference. The Ti6Al4V powder was observed to have conducted heat faster to its neighbouring particles than the SS316L powder. The thermal conductivity of Ti6Al4V was twice as much as SS316L. Hence, the heat is able to be conducted twice as fast for Ti6Al4V.

Table 3.3 Volumetric heat capacity of SS316L and Ti6Al4V

Material	Volumetric heat capacity ($\text{MJ m}^{-3} \text{K}^{-1}$)
SS316L	3.70
Ti6Al4V	2.95

Figure 3.5 Temperature profile of SS316L and Ti6Al4V powders at (a) time = 275 μs and (b) 887.5 μs at $x = 200 \mu\text{m}$

3.4 Summary

In this chapter, the powder bed deposition process was modelled for single and multi-material using DEM. The powders follow a Gaussian distribution, similar to the powders used in experiments. The powders were released from a height to allow them to spread randomly on the substrate. A heat source was modelled to travel along the surface of the powders to simulate the laser heating in SLM.

In the single material model, the melt pool width was observed to have significant difference when compared to experimental results. This is due to the absence of heat convection, phase change and vaporization which resulted in the heat being trapped in the powder for a prolonged period. In the multi-material model, the effect of heat conduction was observed between SS316L and Ti6Al4V. As Ti6Al4V has a greater heat conduction coefficient, it was able to conduct heat much faster away from the powder at the surface.

The setback of this model is that it only uses particles and does not account for fluid flow. In SLM process, the flow of the molten metal can affect the formation of the melt track and produce defects such as discontinuous tracks or porosities.

4. Computational Fluid Dynamics Of Single Material SLM Process

4.1 Introduction

In this chapter, the CFD modelling method will be built on the powder bed generated using DEM. A single laser beam was modelled to scan along the y-axis to form a single track. Different scanning parameters were studied to vary the energy density on the powder bed. A key defect in SLM is the presence of porosities in built parts. Porosity can be formed from trapped gases in the melt pool at high scanning speed or due to keyhole instability during rapid solidification of the metal leading to the collapse of the keyhole [111]. Since porosity is embedded within the part, it is difficult to detect as opposed to balling. These defects will result in parts with lower mechanical properties [112]. In-situ monitoring of the melt pool allows the user to detect defects in real-time and pause the printing process to make adjustments [115, 116]. Non-destructive testing (NDT) methods such as radiography can be used to monitor the quality of the printed part [113]. Experiments revealed that porosity can be controlled by using suitable energy density and modifying the parameters in Equation 4.1 if required [114, 115].

The energy density E , which is the applied energy per volume of material, is given by [116, 117, 118]

$$E = \frac{P}{v \cdot h \cdot L} \quad (4.1)$$

where P is the laser power, v is the laser scanning speed, h is the hatch spacing and L is the layer thickness.

A study on the effects of the energy density on the porosities of the melt track was performed and compared to observations in experiments. The CFD model allows a better understanding on the formation of different types of porosities as the model is able to provide information of the flow behaviour of the molten metal during the melting and solidification process.

4.2 Methodology

Using DEM, the shapes of the powders are set to be spherical and their sizes follow a Gaussian distribution with mean diameter of $27\text{ }\mu\text{m}$ ($D_{50} \approx 27\text{ }\mu\text{m}$) and a full width at half maximum value of $5\text{ }\mu\text{m}$. The powders were released from a height of $700\text{ }\mu\text{m}$ to allow for random dispersion of the powder. Every powder's radii and coordinates were then exported to OpenFOAM® software to generate the powders and their location on the substrate, and to perform CFD simulation work. The timestep was set at 10 ns and a Cartesian mesh grid size of $2.5\text{ }\mu\text{m}$ was used. A laser beam diameter of $54\text{ }\mu\text{m}$ and layer thickness of $27\text{ }\mu\text{m}$ were used for the simulations. A single track of $800\text{ }\mu\text{m}$ in length was scanned for each of the three sets of parameters used for this study. The initial temperatures of the powders and substrate were set to 300 K and the boundary conditions were assumed to be adiabatic.

To compare the effects of different energy densities on the melt track, three sets of parameters were used as shown in Table 4.1. They are classified based on their energy densities. For a single track, the energy density, E , was calculated using Equation 4.1 while setting the hatch spacing to be equivalent to the laser beam diameter.

Table 4.1. Parameters used in simulations ($h = 54 \text{ } \mu\text{m}$, $L = 27 \text{ } \mu\text{m}$)

Runs	Laser power (W)	Scanning speed (m s^{-1})	E (J mm^{-3})
Low	75	1.5	34.3
Medium	200	1.5	91.4
High	400	1.5	182.9

4.2.1 Heat transfer and fluid flow

In the model, metallic and gas phases were used to show the evolution of the interface during the melting and solidification process in SLM. To capture the metal and gas interface, the volume of fluid (VOF) method was adopted. In the model, a function was used to determine the metallic and gaseous phase α_1 and α_2 respectively. The relationship between these phases can be defined as [85]

$$\alpha_1 + \alpha_2 = 1 \quad (4.2)$$

When $\alpha_1 = 1$, the mesh consists of only metallic phase. Likewise, when $\alpha_2 = 1$, the mesh consists of solely gas. When the solid metal powders experience melting, it will change from solid to liquid state. This change in phase is described using the liquid fraction γ . It follows a linear function ranging from zero to one, where the value of zero means the metal is completely solid while the value of one means the metal is fully liquid [119]. When γ is between zero and one, the metal is in a mushy state.

The molten metal was assumed to be an incompressible fluid. This means that for a selected volume, the amount of fluid entering it is equivalent to the amount of fluid

exiting. Hence, the continuity equation expressing the conservation of mass can be written as

$$\nabla \cdot \vec{u} = 0 \quad (4.3)$$

where $\vec{u}$ is the flow velocity. The forces acting on the system during the SLM process were considered in the Navier-Stokes or the conservation of momentum equation. Equation 4.4 shows the pressure forces on the left-hand side being driven by the external forces on the right hand side of the equation, giving

$$\begin{aligned} \frac{\partial \bar{\rho} \vec{u}}{\partial t} + \nabla \cdot (\bar{\rho} \vec{u} \otimes \vec{u}) = & -\nabla p + \nabla \cdot (\bar{\mu} \cdot \nabla \vec{u}) + \bar{\rho} g \hat{e}_z \beta (T - T_{ref}) - K_c \left[\frac{(1-\gamma)^2}{\gamma^3 + C_k} \right] \vec{u} \\ & + \left\{ \sigma \kappa \vec{n} + \frac{d\sigma}{dT} [\nabla T - \vec{n} (\vec{n} \cdot \nabla T)] + p_v \right\} |\nabla \alpha_1| \frac{2\bar{\rho}}{(\rho_{metal} + \rho_{air})} \end{aligned} \quad (4.4)$$

where $\bar{\rho}$ is the density, ρ_{metal} is the density of the metal, ρ_{air} is the density of air, t is the time, $\bar{\mu}$ is the viscosity, T is the temperature, T_{ref} is the reference temperature, p is the pressure, g is the gravitational acceleration, p_v is the recoil pressure, $\hat{e}_z$ is the unit normal to the gravitational force, β is the thermal expansion coefficient, K_c is the permeability coefficient, C_k is a constant, σ is the surface tension and κ is the surface curve at unit normal to $\vec{n}$. $|\nabla \alpha_1|$ was used to transform a surface force per unit area into a volumetric surface force [120, 121].

$K_c \left[\frac{(1-f_l)^2}{f_l^3 + C_k} \right] \bar{u}$ is the Carman-Kozeny equation derived from the Darcy's Law

[122]. It describes the flow in the mushy region of the molten pool. The constant C_k was introduced to avoid division by zero and was set to be a small value.

$\frac{d\sigma}{dT} [\nabla T - \vec{n}(\vec{n} \cdot \nabla T)]$ describes the Marangoni force or thermo-capillary force that varies with temperature. Marangoni shear force is attributed to the gradient of surface tension at the gas/metal interface. Surface tension of a material is temperature dependent. Therefore, the temperature gradient of a melt pool can lead to the change of surface tension at the interface, which causes the Marangoni shear force. Studies have shown that it strongly affects the flow pattern in a melt pool [123].

In laser melting process, the temperature within the laser beam will exceed the boiling point of the material. In such a situation, the metal will vaporize and exert a pressure known as recoil pressure p_v on the surface of the molten pool. This will form a depression at the leading edge of the melt track. The equation for recoil pressure is given by [124]

$$p_v = 0.54 p_0 \exp \left(\Delta H_v M \frac{T - T_{LV}}{RT T_{LV}} \right) \quad (4.5)$$

where p_0 is the atmospheric pressure, ΔH_v is the latent heat of vaporization, M is the molar mass, R is the universal gas constant and T_{LV} is the boiling temperature at atmospheric pressure.

In the system, there are energy input from the laser source as well as the heat losses due to conduction, convection and radiation. Change in phase (solid to liquid) of the

metal during melting will require energy from the system, known as the latent heat of fusion. These processes are included in the conservation of energy equation given by

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{C}_p T}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{C}_p T) = & -\frac{\partial \bar{\rho} \Delta H_f}{\partial t} - \nabla \cdot (\bar{\rho} \bar{u} \Delta H_f) + \nabla \cdot (\bar{k} \nabla T) + Q_T \\ & - \left[h_c (T - T_{ref}) + \sigma_s \varepsilon (T^4 - T_{ref}^4) + Q_v \right] \end{aligned} \quad (4.6)$$

$$|\nabla \alpha_1| \frac{2 \bar{C}_p \bar{\rho}}{C_{p-metal} \rho_{metal} + C_{p-air} \rho_{air}}$$

where $C_{p-metal}$ is the specific heat of the metal, C_{p-air} is the specific heat of air, $\bar{C}_p$ is the specific heat, ΔH_f is the enthalpy change due to fusion, $\bar{k}$ is the thermal conductivity, h_c is the heat transfer coefficient, σ_s is the Stefan-Boltzmann constant, ε is the emissivity, Q_v is the heat loss due to evaporation, and Q_T is the heat input.

The heat loss due to conduction, convection and radiation are given by $\nabla \cdot (\bar{k} \nabla T)$,

$h_c (T - T_{ref})$ and $\sigma_s \varepsilon (T^4 - T_{ref}^4)$ respectively. The term $-\frac{\partial \bar{\rho} \Delta H_f}{\partial t} - \nabla \cdot (\bar{\rho} \bar{u} \Delta H_f)$

represents the change in enthalpy due to the change in metallic phase.

Due to the high temperature of the molten metal during the melting process, surface evaporation at the molten pool may arise. This will result in loss of energy to convert the metal from liquid to gaseous phase and is expressed as

$$Q_v = 0.82 \frac{\Delta H_v M}{\sqrt{2\pi MRT}} p_0 \exp \left(\Delta H_v M \frac{T - T_{LV}}{RT T_{LV}} \right) \quad (4.7)$$

The laser beam intensity I can be approximated as a Gaussian distribution given by

$$I = \frac{2\eta P}{\pi r^2} \exp \left[-2 \frac{(x - x_0)^2 + (y + v \cdot t - y_0)^2}{r^2} \right] \quad (4.8)$$

where η is the absorptivity coefficient, P is the laser power, x and y are the cartesian coordinates of the centre of the laser beam at time t . x_0 and y_0 are the starting coordinates of the laser beam, r is the radius of the laser beam and v is the scanning speed. The radius of the laser beam for the simulation is set to be $27 \mu\text{m}$ and the absorptivity was taken to be 0.35.

To obtain the laser beam energy density, the intensity of the beam was divided by the depth of the heat source and can be expressed by

$$Q_T = \frac{I \cdot f_{\text{absorb}}}{\Delta z} \quad (4.9)$$

where Δz represents the height of the numerical grid and f_{absorb} is an indicator ranging from 0 to 1 to ensure the heat flux is only applied on the top surface of the metal. In this model, the Fresnel reflection was neglected due to the high computational cost.

4.2.2 Modelling of laser absorption

The laser beam was discretized as bundles of laser rays that are directly absorbed by the top surface of the metallic phases. A dimensionless variable, f_{absorb} , ranging from 0 to 1, was introduced to track the top surface of the metal. Figure 4.1 shows part of the metal powder with the heat source travelling from the top row to the bottom row. The sum of f_{absorb} for each column cannot be more than 1 to ensure that the amount

of heat energy absorbed by the column will not exceed the heat energy entering the column. The calculation of f_{absorb} for each cell depends on the volume fraction of metallic phases.

In column 2 of Figure. 4.1, row 1 and row 2 consist of gaseous phase ($\alpha_1 = 0$), therefore f_{absorb} for the two cells are 0 and no heat energy is absorbed by the cells. When the heat source reaches the first cell with metallic phase ($\alpha_1 \neq 0$), f_{absorb} will take on the value of the corresponding α_1 . Therefore, in row 3, α_1 has a value of 0.4 and the value of f_{absorb} will be updated to 0.4. In row 4, the cell has only metallic phase and hence, α_1 has a value of 1. However, f_{absorb} was set as 0.6 to ensure the sum of f_{absorb} for the column is less than or equal to 1. Table. 4.2 shows the values of f_{absorb} for column 2.

In column 3, row 1 has only the gaseous phase ($\alpha_1 = 0$) and the corresponding f_{absorb} for the cell is 0. Row 2 has an α_1 value of 0.05 and f_{absorb} value will be set as 0.05. In row 3, the cell has an α_1 value of 0.94 and the f_{absorb} value for the cell will be set as 0.94. Row 4 consist of only the metallic phase and its α_1 value will be 1.0. However, f_{absorb} will be 0.01. Table. 4.3 shows the values of f_{absorb} for column 3.

Such implementation of f_{absorb} was employed to ensure that the heat flux is only applied at the top surface of the workpiece.

Figure 4.1 Mesh cells showing part of a metal powder. The blue regions represent the metallic phases while the white regions represent the gaseous phases.

Table 4.2 Values of f_{absorb} for Column 2

Row	1	2	3	4	5
α_1	0	0	0.4	1.0	1.0
f_{absorb}	0	0	0.4	0.6	0

Table 4.3 Values of f_{absorb} for Column 3

Row	1	2	3	4	5
α_1	0	0.05	0.94	1.0	1.0
f_{absorb}	0	0.05	0.94	0.01	0

4.2.3 Material properties

The material used for the simulations is SS316L. The material properties, coefficients and constants are listed in Table 4.4 [127, 128, 129]. In the simulation, the material's properties are temperature dependent that provides a better representation of the properties of the mushy region.

Table 4.4. Physical properties for SS316L used in simulations.

Physical Properties	Values
Solidus temperature (K)	1658
Liquidus temperature (K)	1723
Boiling temperature (K)	3090
Surface tension (N m^{-1})	1.6
Coefficient of surface tension ($\text{N m}^{-1} \text{K}^{-1}$)	8×10^{-4}
Base thermal conductivity of solid ($\text{W m}^{-1} \text{K}^{-1}$)	9.248
Base thermal conductivity of liquid ($\text{W m}^{-1} \text{K}^{-1}$)	12.41
Reference temperature (K)	300
Base density of liquid (kg m^{-3})	7433
Base density of solid (kg m^{-3})	8084
Specific heat of solid metal ($\text{J kg}^{-1} \text{K}^{-1}$)	462
Specific heat of liquid metal ($\text{J kg}^{-1} \text{K}^{-1}$)	775
Latent heat of fusion (J kg^{-1})	2.7×10^6
Latent heat of vaporization (J kg^{-1})	7.45×10^6
Emissivity	0.26
Convective coefficient ($\text{W m}^2 \text{K}$)	80
Darcy term coefficient ($\text{kg m}^{-3} \text{s}^{-1}$)	1×10^6
Stefan-Boltzmann's constant ($\text{W m}^{-2} \text{K}^{-4}$)	5.67×10^{-8}
Universal gas constant ($\text{J K}^{-1} \text{mol}^{-1}$)	8.3144
Atmospheric pressure (N m^{-2})	101000
Molar Mass (kgmol^{-1})	0.05593

The density of metal in the mushy state is given by

$$\begin{aligned} \rho_{metal} = & \gamma \left(\rho_{liquid} + 0.0393T + 0.00018T^2 \right) \\ & + (1-\gamma) \left(\rho_{solid} - 0.4209T - 3.984 \times 10^{-5}T^2 \right) \end{aligned} \quad (4.10)$$

where ρ_{liquid} is the base value for the density of the metal in liquid state and ρ_{solid} is the base value for the density of the metal in solid state.

The thermal conductivity of the metal is given by

$$\lambda_{metal} = \gamma \left(\lambda_{liquid} + 0.003279T \right) + (1-\gamma) \left(\lambda_{solid} - 0.1571T \right) \quad (4.11)$$

where λ_{liquid} is the base value for the density of the metal in liquid state and λ_{solid} is the base value for the density of the metal in solid state.

The dynamic viscosity, μ , of the metal is given by [125]

$$\lg(\mu) = \frac{2385.5}{T} - 3.5958 \quad (4.12)$$

The unit of μ is Pa.s. The corresponding dynamic viscosity at liquidus temperature (1723 K) is 6.15×10^{-3} Pa.s.

To calculate the properties of a single mesh, the generic equation is computed as

$$\phi = \phi_{metal} \cdot \alpha_1 + \phi_{air} \cdot \alpha_2 \quad (4.13)$$

where ϕ_{air} is the selected material property of the gas and ϕ_{metal} is the selected property of the metal. Therefore, the thermal conductivity of the mesh is $\lambda_{metal} \cdot \alpha_1 + \lambda_{air} \cdot \alpha_2$.

4.3 Results and discussions

To validate the model, a comparison of the melt pool's characteristics was performed between the simulation and experimental results by Kamath et al. [110]. Table. 4.5 shows the melt pool's width and depth obtained using the model. From the comparisons, it can be observed that the simulation measurements are in line with the experiment measurements with an error of up to 7.9 %. Cross-sections of the melt pools simulations are shown in Figure 4.2.

Table 4.5. Comparison of width and depth of simulations with constant scanning speed of 1.5 m/s with experimental data [112].

Laser Power (W)	Width (μm)			Depth (μm)		
	Simulation	Experiment	Error (%)	Simulation	Experiment	Error (%)
200	80	84	4.8	52.5	57	7.9
300	77.5	83	6.6	95	94	1.1
400	100	103	2.9	115	119	3.4

Figure 4.2 Cross-sections of melt pools using scanning speed of 1.5 m/s and laser powers of (a) 200 W, (b) 300 W and (c) 400 W. The red region shows the material which was melted and solidified during the SLM process.

4.3.1 Single track formation during SLM

Figure 4.3 Melt track using $P = 200$ W, $v = 1.5$ m/s (a) Top view, sliced at (b) $x = 100$ μm , and (c) $x = 125$ μm .

Using a scanning speed of 1.5 m/s and laser power of 200 W, the evolution of temperature field and geometry of the melt track are shown in Figure 4.3. It can be clearly seen that a continuous and relatively smooth track is formed due to the fusion of metal particles. As shown in Figure 4.3, metal particles near and within the laser beam spot were irradiated, heated up and melted. Due to the surface tension force, those melted particles immediately coalesce with nearby powders and the substrate, leading to the formation of a track. In addition, an obvious depression zone, attributed to the recoil pressure, can be observed near the laser beam spot. The metal at the centre of the laser beam will reach temperatures above its boiling point leading to evaporation of the metal. This metal vapour exerts a force which results in the depression observed at the leading edge of the melt pool. Such phenomenon is in agreement with previous experimental study [126]. The local temperature quickly drops as the laser beam moves away and this results in a drop in evaporation rate of the metal. This leads to a rapid decrease of the recoil pressure force. In this situation, the surface tension starts to dominate the dynamics of fluids, resulting in the motion of fluid towards the centre of the depression zone. The reverse motion of liquid melts causes the collapse (or recovery) of the depression zone. The keyhole maintains its profile when the recoil pressure balances with the surface tension as shown in experiments, giving a constant depth throughout the scanning process [126]. As illustrated in Figure 4.3(b), a thin liquid layer can be observed in the front of the depression zone, which is consistent with previous study [127]. Moreover, the keyhole depression at the end of the track retains its shape despite after the heat source is turned off and is attributed to the fast cooling and solidification near the depression zone. Similar observation has also been reported by laser welding experiments where

Eriksson et al. studied the inclination of the keyhole front [128]. One may also find such characteristics in SLM experiments [129] and it was reported that a depression zone is formed at the end of the melt track.

The longitudinal 2D slices of the model in Figure 4.3(b) and (c) are employed to determine whether any porosity is formed after the laser scanning. Similar operation has been conducted by SLM experiments to show the distribution of porosity [85]. In Figures 4.3(b) and (c), the cross-sectional slices were taken at $x = 100 \mu\text{m}$ (corresponding to the centre of the laser beam) and $x = 125 \mu\text{m}$ (near the inside edge of the laser beam), respectively. Since $x = 125 \mu\text{m}$ falls within the region covered by the laser beam spot, full melting of the powders should be observed when sufficient energy density is applied. This corresponds to experiments where the track widths of a continuous single track are larger than the diameter of the laser spot [130, 131]. As shown in Figure 4.3, no porosity could be observed below the solidified track, indicating the applied laser parameters are suitable in preventing the development of porosities. Additionally, Figure 4.3(b) and (c) provide information about the surface roughness of the solidified track. The track is relatively smooth as shown in the figures. As discussed by Zhou et al. [132], a smooth surface is significant in eliminating interlayer porosities from building up in the next layer. On the contrary, a rough surface will affect the powder distribution across the layer and deteriorates laser absorptivity.

4.3.2 Formation of irregular pores

Irregular pores are often observed in experiments when using parameters of lower energy densities (high scanning speed and/or low laser power) than the optimal values [111, 133]. At high scanning speed, balling effects occurs and gives rise to discontinuous tracks and pores trapped between these balls [90]. In the subsequent layers, the molten metal flow is disturbed due to the unevenness of the preceding layer and is unable to fill up the pores left behind from the previous layers. To simulate porosity from the lack of energy density, a low laser power of 75 W was adopted. The scanning speed was retained at 1.5 m/s, thus reducing the total energy density by more than two times according to Equation 4.1.

Figure 4.4 Melt pool track using low laser power $P = 75 \text{ W}$, $v = 1.5 \text{ m/s}$ (a) top view, sliced at (b) $x = 100 \mu\text{m}$ and (c) $x = 125 \mu\text{m}$.

In Figure 4.4(a), it was observed that the track width is narrower than that in Figure 4.3(a). Lower laser power will produce a smaller melt pool since lesser energy was used to melt the powders. This can be seen in Figure 4.4(b) where the molten track has a shallower depth than that in Figure 4.3(b). In Figure 4.4(c), it was also observed that the powders that are within the laser beam diameter did not experience full melting that contributes to a smaller molten pool. With a smaller molten pool, there is insufficient molten metal to flow and fill up the gaps between the powders. Therefore, pores are formed and will take on irregular shapes from these gaps as seen in Figure 4.4(c). These are similar to experimental results reported in Aboulkhair's et al. work [111]. Since the powders were poorly melted, they will not adequately fuse with the substrate. This will result in poor interlayer bonding leading to delamination defects seen in experiments with low energy density parameters [134].

Additionally, from Table 4.6, the melt pool depth was measured to be 10 μm which is less than the layer thickness of the simulation. For the laser to remelt the layer directly beneath the current layer, the melt pool depth will have to be more than the layer thickness. When a new layer of powders is deposited, the laser will therefore not be able to completely melt the layer beneath it. With insufficient melting, there will not be enough molten metal to fill up the porosities from the previous layer. Hence, the shapes and positions of these porosities due to the lack of fusion are unaffected by the scanning process of the subsequent layers.

Table 4.6. Melt pools' width and depth from simulation results.

Runs	Width (μm)	Depth (μm)
Low	60	10
Medium	80	52.5
High	100	115

4.3.3 Formation of spherical pores

Previous experiments reported that low scanning speed and high laser energy input resulted in the formation of porosities [135]. Therefore, a high laser power of 400 W and the same scanning speed of 1.5 m/s were employed to study the formation of pores.

Increased porosities in SLM parts was observed when using energy density above the optimal range [111]. With higher energy density applied on the powder bed, the temperature of the melt pool will increase that leads to more vaporized metal and increased recoil pressure. These result in deeper and unstable keyhole being formed [136]. Due to its instability, the keyhole will collapse, trapping gas within the melt pool. The increase in recoil pressure also leads to more molten metal being pushed to the sides of the tracks as seen in Figure 4.5(a). Increasing the energy density will lead to an increase in the keyhole depth as seen in Figure 4.5(b) and (c) when compared to that in Figure 4.3(b) and (c).

Figure 4.5 Melt pool track using high laser power, $P = 400 \text{ W}$, $v = 1.5 \text{ m/s}$ (a) top view, sliced at (b) $x = 100 \mu\text{m}$ and (c) $x = 125 \mu\text{m}$.

In Figure 4.6, the formation of the pores can be studied. As the keyhole travels along the scanning direction, the molten metal trailing it will attempt to fill up the vacancy. Due to Marangoni convection, the molten metal at Region A will flow away from the keyhole shown by its resultant velocity vector [137]. At the same time, the molten metal in Region B will collapse inwards towards the keyhole due to surface tension. With the bottom and top of the molten metal having different flow directions, the molten metal will enclose and trap the gas within the keyhole. This gas consists mainly the metal vapour trying to escape from the bottom of the keyhole [136]. The cross-section along the track's length showed similar characteristics when compared with experiments by King et al. [135]. The majority of the keyhole porosities were located near the bottom of the keyhole as shown in Figure 4.5(b) and (c). From Figure

4.5, the velocities of the tailing end of the keyhole, in Region B, can reach up to 5 m/s. This rapid flow of the molten metal to fill the keyhole will give insufficient time for the gas to escape from the collapsing keyhole.

Figure 4.6 Velocity vectors of molten metal around the keyhole at $x = 100 \mu\text{m}$.

Figure 4.7 shows the cross-sections of the melt pool in the x -axis using laser power of 400 W and scanning speed of 1.5 m/s. The formation of a pore was observed from the time when the keyhole began to collapse until the time when the molten metal trapped the gas bubble. In Figure 4.6, the molten metal near the surface is flowing rapidly to fill up the keyhole. However, the molten metal near the base of the keyhole was flowing away from the keyhole as seen in Region A of Figure 4.6. This leads to gas being trapped as seen in Figures 4.7(b) and (c). Within the molten metal, the trapped gas will take on an elliptical or spherical shape due to the effects of surface

tension as seen in Figure 4.7(d). Due to surface tension, the molten metal will be pulled towards each other, minimizing the surface area of the liquid-gas interface. These corresponds to experimental results reported by King et al. [135].

Figure 4.7 Cross-section of powder bed at $x = 95 \mu\text{m}$ showing evolution of a keyhole porosity in the molten metal starting with (a) the unstable keyhole beginning to collapse at time = 266 μs , (b) trapping of gas within the molten metal at time = 270 μs , (c) molten metal enclosing the gas forming pores at time = 272 μs and (d) spherical pores formed due to surface tension at time = 282 μs .

From Table 4.6, the keyhole depth of 112.5 μm exceeds the layer thickness of 27 μm . Therefore, in the subsequent layers, the keyhole will be able to reach the existing pores due to the deep penetration depth of the laser. This will remelt the metal from the previous layer(s) and remove any existing pores that are within reach of the keyhole. However, the keyhole is unstable and will result in the formation of new

keyhole pores. Therefore, the keyhole porosities may change their sizes and locations after the scanning of every layer.

4.4 Summary

Different energy density parameters were studied to observe the effects they have on pore formation. The parameters using laser power of 200 W and scanning speed of 1.5 m/s were chosen as a reference for comparisons. Energy densities lower and higher than this reference were used in the simulations to study the differences between the pores formed in each scenario. Pores were formed when using too low or too high energy density parameters. In the reference parameters, sufficient energy was used to melt the metal powders and the keyhole remained stable with no pores observed. However, when low scanning speed was used, the pores were formed due to the incomplete melting of the powders, leaving gaps between the partially melted powders.

Similarly, pores were formed when high energy density parameters were used. The collapse of the unstable keyhole was due to the high velocities of the molten metal near the surface flowing back to fill up the keyhole while the molten metal near the base of the keyhole was flowing away from the keyhole because of the recoil pressure. The flow velocity and direction of the molten metal can be shown using this simulation to explain the formation of keyhole porosities. The gas near the bottom are more likely to be trapped from the collapsing keyhole. Therefore, most of the keyhole porosities are formed near the base of the keyhole. The shapes of these pores take on an elliptical or spherical shape due to the effect of surface tension.

The porosities characteristics in the simulations fits those found in experiments. In Kasperovich et. al works, their experimental results closely resembles the simulation results presented in this chapter [138]. They experimented on three different energy densities to find out their effects on the porosities. Using tomography, they were able to determine the shapes of the porosities present in the samples. In their experiments, the sample printed using the lowest energy density has highly irregular shape pores while the sample printed using the highest energy density has pores that have high sphericity.

This physics-based model has given a clearer understanding of the formation of pores during the melting and solidification process. This chapter established that the porosities' characteristics vary when using different parameters. It also provides an illustration and explanation on the mechanics behind the formation of keyhole porosity.

5. Computational Modelling Of Multi-Material In SLM Process

5.1 Introduction

In this chapter, multi-material modelling will be discussed. The multi-material model is built on the model described in chapter 4. An additional α phase was included in the governing equations to represent the second metal.

In a multi-material model, there is interaction between two liquid metals due to surface tension. This is similar to the surface tension of a single metal where it interacts with the atmosphere. For two liquids, the surface tension can be referred to as the interfacial tension. While there are instruments to measure the surface tension of liquid metals in atmosphere medium, there is currently no instruments able to measure the interfacial tension between two liquid metals. This chapter will focus on the methodology for a multi-material SLM simulation and the study on the impact of different interfacial tensions on the resultant melt pool formation.

5.2 Methodology

DEM was used to generate powders of different materials. Each material was represented by a phase fraction, α . Their relationship can be established by a generic equation computed as

$$\sum_{i=1}^n \alpha_i = 1 \quad (5.1)$$

where n is the number of materials present in the simulation. In this chapter, there are two metallic phases and a gaseous phase present in the model, hence n is 3. The metals will be identified as metal 1 and metal 2 to facilitate the explanation of the model. The VOF of metal 1 will be α_1 and the VOF of metal 2 will be α_2 .

In this model, a volume weighted average method was introduced to determine the contribution of fluid forces from each liquid metal based on their ratios. In chapter 4, there is only one metallic phase in the model. Therefore, the fluid forces such as Marangoni force, surface tension and recoil pressure acting on the liquid metal were attributed to the material properties of the single metal. However, in a multi-material model, each of these forces are calculated based on the ratio of individual liquid fraction of the metals. In Figure 5.1(a), the cell consists of only liquid metal 1. Therefore, all the fluid forces acting on the cell is only due to the material properties of liquid metal 1. In Figure 5.1(b), the cell consists of half of liquid metal 1 and half of liquid metal 2. Hence, each liquid metal will contribute to half of the total fluid forces acting on the cell.

Figure 5.1 Cell mesh with (a) only liquid metal 1 and (b) half of liquid metal 1 and half of liquid metal 2

The volume weighted average of liquid metal 1 and 2 are

$$w_1 = \frac{\alpha_1 \gamma_1}{\alpha_1 \gamma_1 + \alpha_2 \gamma_2 + C_k} \quad (5.2)$$

$$w_2 = \frac{\alpha_2 \gamma_2}{\alpha_1 \gamma_1 + \alpha_2 \gamma_2 + C_k} \quad (5.3)$$

where γ_1 is the liquid fraction of metal 1, γ_2 is the liquid fraction for metal 2 and C_k is a constant of small value to avoid division by zero.

To calculate the material property of a single mesh, a general equation can be used and it is given by

$$\phi = \phi_{metal} \cdot (\alpha_1 + \alpha_2) + \phi_{air} \cdot \alpha_3 \quad (5.4)$$

where ϕ_{air} is the selected material property of the gas and ϕ_{metal} is the selected material property of the metals.

ϕ_{metal} can be represented by volume weighted average of metal 1 and metal 2, given by

$$\phi_{metal} = \phi_{metal.1} \cdot \frac{\alpha_1}{\alpha_1 + \alpha_2 + C_k} + \phi_{metal.2} \cdot \frac{\alpha_2}{\alpha_1 + \alpha_2 + C_k} \quad (5.5)$$

where $\phi_{metal.1}$ is the selected property of metal 1 and $\phi_{metal.2}$ is the selected property of metal 2.

5.2.1 Governing Equations

The conservation of mass for multi-materials model is given by

$$\nabla \cdot \vec{u} = 0 \quad (5.6)$$

and the conservation of momentum equation is given by

$$\begin{aligned}
\frac{\partial \bar{\rho} \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) = & -\nabla p + \nabla \cdot (\bar{\mu} \cdot \nabla \bar{\mathbf{u}}) + \bar{\rho} g \bar{e} \beta_{metal} (T - T_{ref}) \\
& - w_1 \cdot K_{c1} \left[\frac{(1-\gamma_1)^2}{\gamma_1^3 + C_k} \right] \bar{\mathbf{u}} - w_2 \cdot K_{c2} \left[\frac{(1-\gamma_2)^2}{\gamma_2^3 + C_k} \right] \bar{\mathbf{u}} \\
& + \left\{ w_1 \cdot \frac{d\sigma_1}{dT} [\nabla T - \bar{\mathbf{n}} (\bar{\mathbf{n}} \cdot \nabla T)] + w_2 \cdot \frac{d\sigma_2}{dT} [\nabla T - \bar{\mathbf{n}} (\bar{\mathbf{n}} \cdot \nabla T)] \right. \\
& \left. + p_v \right\} |\nabla (\alpha_1 + \alpha_2)| \frac{2\bar{\rho}}{(\rho_{metal} + \rho_{air})} + \bar{\mathbf{f}}_{st}
\end{aligned} \tag{5.7}$$

where β_{metal} is the thermal expansion coefficients of the metals, K_{c1} is the permeability coefficient of metal 1, K_{c2} is the permeability coefficient of metal 2,

$\frac{d\sigma_1}{dT}$ is the thermal coefficient of surface tension of metal 1, $\frac{d\sigma_2}{dT}$ is the thermal

coefficient of surface tension of metal 2 and $\bar{\mathbf{f}}_{st}$ is the surface tension forces.

$|\nabla (\alpha_1 + \alpha_2)|$ was used to transform a surface force per unit area into a volumetric surface force.

The surface tension forces are given by [139]

$$\bar{\mathbf{f}}_{st} = \sigma \kappa \bar{\mathbf{n}} \tag{5.8}$$

where σ is the surface tension coefficient, κ is the curvature to the unit normal vector $\bar{\mathbf{n}}$ of the interface.

The recoil pressure, p_v , is given by

$$p_v = w_1 \cdot 0.54 p_0 \exp \left(\frac{\Delta H_{v1} M_1}{RT T_{LV1}} \frac{T - T_{LV1}}{T} \right) + w_2 \cdot 0.54 p_0 \exp \left(\frac{\Delta H_{v2} M_2}{RT T_{LV2}} \frac{T - T_{LV2}}{T} \right) \tag{5.9}$$

where p_0 is the atmospheric pressure, ΔH_{V1} is the latent heat of vaporization of metal 1, ΔH_{V2} is the latent heat of vaporization of metal 2, M_1 is the molar mass of metal 1, M_2 is the molar mass of metal 2, R is the universal gas constant, T_{LV1} is the boiling temperature of metal 1 at atmospheric pressure and T_{LV2} is the boiling temperature of metal 2 at atmospheric pressure.

The conservation of energy equation is given by

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{C}_p T}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{C}_p T) = & -\frac{\partial \bar{\rho} \Delta H_f}{\partial t} - \nabla \cdot (\bar{\rho} \bar{u} \Delta H_f) + \nabla \cdot (\bar{k}_{metal} \nabla T) + Q_T \\ & - \left[h_{c-metal} (T - T_{ref}) + \sigma_s \varepsilon_{metal} (T^4 - T_{ref}^4) + Q_v \right] \quad (5.10) \\ & \left| \nabla (\alpha_1 + \alpha_2) \right| \frac{2 \bar{C}_p \bar{\rho}}{C_{p-metal} \rho_{metal} + C_{p-air} \rho_{air}} \end{aligned}$$

where $\bar{k}_{metal}$ is the thermal conductivity of the metals, $h_{c-metal}$ is the heat transfer coefficient of the metals and ε_{metal} is the emissivity of the metals.

The heat loss due to evaporation can be expressed as

$$\begin{aligned} Q_v = & w_1 \cdot 0.82 \frac{\Delta H_{V1} M_1}{\sqrt{2\pi M_1 R T}} p_0 \exp \left(\Delta H_{V1} M_1 \frac{T - T_{LV1}}{R T T_{LV1}} \right) \\ & + w_2 \cdot 0.82 \frac{\Delta H_{V2} M_2}{\sqrt{2\pi M_2 R T}} p_0 \exp \left(\Delta H_{V2} M_2 \frac{T - T_{LV2}}{R T T_{LV2}} \right) \quad (5.11) \end{aligned}$$

The laser beam intensity I can be approximated as a Gaussian distribution given by

$$I = \frac{2\eta_{metals} P}{\pi r^2} \exp \left[-2 \frac{(x - x_0)^2 + (y + v \cdot t - y_0)^2}{r^2} \right] \quad (5.12)$$

where η is the absorptivity coefficient of the metals, P is the laser power and x and y are the cartesian coordinates of the centre of the laser beam at time t . x_0 and y_0 are the starting coordinates of the laser beam, r is the radius of the laser beam and v is the scanning speed. The radius of the laser beam for the simulation is set to be 40 μm .

To obtain the laser beam energy density, the intensity of the beam was divided by the depth of the heat source and can be expressed by

$$Q_T = \frac{I \cdot f_{absorb}}{\Delta z} \quad (5.13)$$

where Δz represents the height of the numerical grid and f_{absorb} is an indicator ranging from 0 to 1 to ensure the heat flux is only applied on the top surface of the metal. In this multi-material model, the f_{absorb} term will consider the additional metallic phase.

Figure 5.1 shows the blue region representing metal 1 and metal 2 while the white region represents the gaseous phase. In column 2, the first two rows do not have any metallic phases and the f_{absorb} term will have a value of 0 to represent no heat flux is absorbed by the meshes. In column 2, row 3 has a $\alpha_1 + \alpha_2$ value of 0.4. The f_{absorb} term will take on the value of 0.4 to represent 40% of the heat flux is absorbed by the mesh and 60% of the heat flux will be received by the mesh in row 4. In row 4, the mesh is filled with metallic phases and the remaining 60% of the heat flux will be absorbed by the cell, resulting in f_{absorb} having a value of 0.6. The calculations can be shown in Table 5.1.

Figure 5.2 Mesh cells showing part of a metal powder. The blue regions represent the two metallic phases while the white regions represent the gaseous phases.

Table 5.1 f_{absorb} for Column 2

Row	1	2	3	4	5
$\alpha_1 + \alpha_2$	0	0	0.4	1.0	1.0
f_{absorb}	0	0	0.4	0.6	0

5.2.2 Simulation and experimental set up

In this model, the laser beam radius is 40 μm . This is to allow validation of the model with experiments using SLM280HL which has a laser beam diameter of 80 μm . The metals used in this model are SS316L and Ti6Al4V. Their individual material properties are widely studied and hence readily available in literature [83, 140, 141]. Table 5.2 shows the material properties of Ti6Al4V used [128, 147, 148]. The material properties of SS316L can be found in Table 4.4.

Table 5.2. Physical properties for Ti6Al4V used in simulations.

Physical properties	Values
Solidus temperature (K)	1877
Liquidus temperature (K)	1923
Boiling temperature (K)	3133
Surface tension (N m^{-1})	1.525
Coefficient of surface tension ($\text{N m}^{-1} \text{K}^{-1}$)	-0.28×10^{-3}
Thermal conductivity of solid ($\text{W m}^{-1} \text{K}^{-1}$)	21
Thermal conductivity of liquid ($\text{W m}^{-1} \text{K}^{-1}$)	29
Density of liquid (kg m^{-3})	3920
Density of solid (kg m^{-3})	4420
Specific heat of solid metal ($\text{J kg}^{-1} \text{K}^{-1}$)	670
Specific heat of liquid metal ($\text{J kg}^{-1} \text{K}^{-1}$)	730
Latent heat of fusion (J kg^{-1})	2.90×10^5
Latent heat of vaporization (J kg^{-1})	4.7×10^6
Emissivity	0.1536
Convective coefficient ($\text{W m}^2 \text{K}$)	20
Darcy term coefficient ($\text{kg m}^{-3} \text{s}^{-1}$)	1×10^6
Molar mass (kgmol^{-1})	0.446

A $400 \mu\text{m} \times 1000 \mu\text{m} \times 200 \mu\text{m}$ SS316L substrate was modelled with a layer of Ti6Al4V powder deposited on it shown in Figure 5.3. The SS316L substrate is represented by the blue region and the Ti6Al4V is represented by the grey powder.

The powder follows a Gaussian distribution with mean diameter of $27\text{ }\mu\text{m}$ ($D_{50} \approx 27\text{ }\mu\text{m}$) and a full width at half maximum value of $5\text{ }\mu\text{m}$. The mesh size for multi-material simulations was $5\text{ }\mu\text{m} \times 5\text{ }\mu\text{m} \times 5\text{ }\mu\text{m}$ and the timestep was 1 ns .

Figure 5.3 Simulation set up of Ti6Al4V powder (grey) on SS316L substrate (blue)

A laser scanning speed of 1 m/s was used for all the simulations. The laser power used was 400 W while three interfacial tensions between the metals was used: 0 , 0.5 and 1 . The simulation runs are shown in Table 5.3. A single track of $800\text{ }\mu\text{m}$ was scanned along the positive y -direction. Interfacial tension values of 0 , 0.5 and 1

N m^{-1} were chosen to study how increasing interfacial tension will affect the melt pool.

Table 5.3 Simulation runs with laser power of 400 W, laser scanning speed of 1 m/s and different interfacial tensions

Runs	Interfacial tension between SS316L and Ti6Al4V (N m^{-1})
1	0
2	0.5
3	1

The experiment was conducted using SLM280HL from SLM Solutions Group AG. A $100 \text{ mm} \times 100 \text{ mm} \times 10 \text{ mm}$ SS316L plate was used as the substrate. Single tracks using 300 W and 400 W were scanned at 1 m/s. The tracks were wire-cut and polished to examine their melt pool geometries under a light optical microscope. Figure 5.4(a) shows the SLM280HL machine, Figure 5.4(b) shows the Ti6Al4V powder on the SS316L substrate before scanning, Figure 5.4(c) shows the single tracks after scanning and Figure 5.4(d) shows the Struers polishing machine used to polish the samples. Figure 5.4(e) shows the Zeiss light optical microscope used to observe cross-section of the melt pool.

Figure 5.4 (a) SLM280HL used for the experiment, (b) interior of SLM machine with Ti6Al4V powder on SS316L substrate, (c) single tracks printed, (d) Struers polishing machine used for polishing surface of melt pool and (e) Zeiss light optical microscope used for observing cross -section of melt pool geometry

5.3 Results and discussions

5.3.1 Validation of model

To validate the model, the melt pool geometries of the simulations was compared to that of the experiments. Figure 5.5(a) and (b) shows the melt pool depth, width and height without interfacial tension between the metals. Figure 5.5(c) shows the cross-section of the melt pool taken using the light optical microscope. Table 5.4 shows the comparisons of the simulation and experimental melt pool geometries. The melt pool

geometries of the simulations with different interfacial tensions were measured to be approximately similar to each other as shown in Table 5.4. This shows that the interfacial tension did not have much impact on the geometries. In this model, the substrate consists of a single material. When the laser penetrates the substrate, the material at the surface of the keyhole comprises mostly SS316L. Hence, the interfacial tension plays a negligible role in the keyhole formation and the depth of the melt pool. The thermal coefficients of surface tension of the materials had different signs. The Ti6Al4V has a negative thermal coefficient of surface tension while the SS316L has a positive term. This will affect their flow directions during the melting process. A negative thermal coefficient of surface tension will result in the Ti6Al4V flowing to the sides of the melt pool while the positive thermal coefficient of surface tension will result in SS316L flowing backwards along the direction of the laser scanning direction [142]. When the two metals are flowing in different

directions, it will reduce the interactions between the metals and the interfacial tensions will therefore play an insignificant role in the formation of the melt pool.

Figure 5.5 Single track cross-sections of simulation with no interfacial tension and experiment using $P = 400\text{ W}$ and $v = 1\text{ m/s}$. The figures show (a) melt pool depth and width of simulation, (b) melt pool height of simulation and (c) melt pool geometry in experiment

Table 5.4 Melt pool geometries of simulations and experiment

Dimension	Simulation with interfacial tension (μm)	Simulation no with 0.5 N m^{-1} interfacial tension (μm)	Simulation with 1.0 N m^{-1} interfacial tension (μm)	Experiment (μm)
Depth	115	115	110	113
Width	125	125	125	136
Height	35	30	30	33

Figure 5.6 Cross-section of melt pool using $P = 400 \text{ W}$, $v = 1 \text{ m/s}$ and interfacial tension $= 1 \text{ N m}^{-1}$. Figures show (a) cross-section of melt pool depth and width, and (b) cross-section of melt pool height

5.3.2 Single track without interfacial tension

For the first simulation, a laser power of 400 W and scanning speed of 1 m/s was used. The interfacial tension between the metals was set to 0 N m⁻¹. In a liquid, molecules exert a cohesive force known as van der Waals' force on their neighbouring molecules [143]. The molecules at the surface experience uneven molecular force and this leads to the molecules at the surface exerting a net inward force towards the liquid shown in Figure 5.7(a). This results in the liquid forming a spherical shape. In the case of two liquids, when the interfacial tension is zero, the molecules of the two liquids exert the same cohesive forces at the interface shown in Figure 5.7(b). The two liquids are miscible and will be able to mix with each other [144]. However, when the interfacial tension is not zero, there is a difference between the forces exerted by the two liquids. The molecule of one liquid will be exerting a greater cohesive force than the molecule of another liquid. This will result in a resultant force and leads to the formation of a spherical droplet.

(a)

(b)

Figure 5.7 (a) Forces acting on molecules in a liquid and on the surface and (b) forces acting on molecules with same cohesive forces at the interface of two liquids

Figure 5.8 shows the time lapses of the formation of the melt track. Figure 5.8(a) shows the powder bed before melting at $t = 0$ s. At $t = 10$ ms, the laser begins to heat and melt the Ti6Al4V powder seen in Figure 5.8(b). Figure 5.8(c) shows the SS316L beginning to melt to form a keyhole. Figure 5.8(d) shows the backward and outward flow of SS316L due to Marangoni effect. Figure 5.8(e) shows the top surface of the melt track consisting of SS316L and Ti6Al4V.

In Figure 5.8(c) and (d), the Ti6Al4V molten metal was observed to be flowing to the sides of the keyhole while the SS316L molten metal was observed to be flowing backwards, away from the keyhole. This can clearly be seen in the cross-section of the melt track in Figure 5.9 showing the SS316L flowing backwards from the keyhole. This is due to the temperature coefficients of surface tension of Ti6Al4V and SS316L. The temperature coefficient of surface tension is negative for Ti6Al4V. This means that the Marangoni convection of Ti6Al4V will be outwards [154, 155]. The flow of the molten Ti6Al4V metal will be away from the centre of the melt pool as seen in Figure 5.10. However, SS316L has a positive temperature coefficient of surface tension and the Marangoni convection of SS316L will be inwards. Therefore, molten SS316L metal will flow towards the centre of the melt pool [156]. This explains the presence of SS316L in the centre of the melt track while Ti6Al4V are observed to be at the sides of the tracks, which are further away from the centre of the melt track. The lack of interfacial tension between the metals resulted in the mixing of the liquid metals at the trailing edge of the melt pool seen in Figure 5.9.

Figure 5.8 Melt track formation with laser scanning with $P = 400$ W and $v = 1$ m/s at (a) $t = 0$ s, (b) $t = 10$ ms, (c) $t = 20$ ms, (d) $t = 80$ ms and (e) $t = 300$ ms. Ti6Al4V is shown in grey and SS316L is shown in blue

Figure 5.9 Cross-section of melt track at $x = 200 \mu\text{m}$. Ti6Al4V is shown in grey and SS316L is shown in blue

Figure 5.10 Cross-section of melt pool. Ti6Al4V is shown in grey and SS316L is shown in blue

5.3.3 Interfacial tensions on melt pool

While the interfacial tension between the metals did not have any impact on the melt pool geometries, it will affect the continuity of the melt track. Figure 5.11 shows the top view and cross-sectional view of the melt track at $x = 200 \mu\text{m}$. In Figure 5.11(a), there is no interfacial tension between the metals. The resultant melt pool shows the two metals were well mixed. The interfaces of the metals were irregular, showing no net forces due to the difference in molecular forces acting on the interfaces.

In Figure 5.11(b), with 0.5 N m^{-1} interfacial tension, the interfaces between the metals tend to be curved due to the interfacial tension. With interfacial tension present, the molecules at the surface of each metals will experience a resultant net force to minimize the interface area between the metals. Figure 5.11(b) shows that the Ti6Al4V forming elliptical shapes when surrounded by SS316L and SS316L forming elliptical shape when it is on Ti6Al4V. Liu et al. and Soysal et al. observed similar occurrence in the steel-copper interface when the metals are immiscible [50, 145]. The steel formed spherical particles in the copper matrix.

Figure 5.11(c) shows the simulation results with interfacial tension of 1 N m^{-1} . Similar to 5.11(b), the Ti6Al4V formed elliptical droplets when surrounded by SS316L. Increasing the interfacial tension resulted in more droplets formed due to greater disparity in the cohesive force between the molecules of the two metals. When the metals formed elliptical droplets on the top surface of the melt track, it will result in the formation of humps. Figure 5.11(c) shows a slight depression at the interfaces of the metals. This will lead to uneven surface finish and give rise to defects.

Figure 5.12 shows an example of an uneven surface finish affecting the subsequent layer. Despite being in the same layer, it can be observed that t_A has a greater depth of unmelted powder when compared to t_B . In such cases, the laser may not be able to penetrate through t_A to fully melt the powders, resulting in pores trapped in between the layers.

Figure 5.11 Top view and cross-sectional view at $x = 200 \mu\text{m}$ of melt track with interfacial tensions: (a) 0 N m^{-1} , (b) 0.5 N m^{-1} and (c) 1 N m^{-1} . Ti6Al4V is shown in grey and SS316L is shown in blue

Figure 5.12 Poor surface roughness affecting the powders thickness across same layer.

5.4 Summary

The methodology and results of a multi-material model has been presented in this chapter. In this model, Ti6Al4V powder was melted on a SS316L substrate with different values of interfacial tensions between the metals. The simulations of the melt pools geometries using 400 W and 1 m/s with different interfacial tensions were compared and validated with experiment results. The melt pool geometries were unaffected by the interfacial tension. The surface of the three keyholes consisted primarily of SS316L, hence, the interfacial tension is negligible in the keyhole region.

In this chapter, the effects of the interfacial tension between the metals were studied. When there is no interfacial tension, the metals are miscible and are able to mix with each other. As interfacial tension increases, the cohesive forces between the metal molecules of individual metals differ and the molecules at the interface experience a net force. This results in the curvature of the liquid metals at the interface observed in the simulations when interfacial tensions were set at 0.5 and 1.0 N m⁻¹.

Experiments using immiscible metals showed similar behaviour of the metals with one metal forming spherical geometry in the matrix of another metal.

The top surface of the melt track was observed to be affected by the interfacial tension. With no interfacial tension, the metals are able to mix and formed a single continuous track. When interfacial tension was introduced, the metals formed elliptical droplets in the matrix of another metal. When the droplets were formed at the surface of the melt track, it resulted in uneven surface of the track observed in the simulation.

This multi-material model has shown the interactions between liquid metals during the SLM process for miscible and immiscible metals. Molecular dynamics can be used to determine the interfacial tension between the metals. This will facilitate in improving the accuracy of the model. Lastly, this model did not consider the chemical behaviour or the solubility of the metals. When miscible metals mix, they can form intermetallic compounds. Current model is unable to show the formation of these intermetallic compounds. When certain liquid metals mix, one of the metals can dissolve in another metal. Current model is unable to account for the solubility of metals. Future work can include the modelling of the intermetallic compounds and incorporate the materials' solubility to improve on this model.

6. Conclusions And Future Works

6.1 Conclusions

This thesis has presented the numerical modelling of the SLM process. DEM was used to model the powder deposition process of the SLM. A Gaussian distribution was used for the powders diameters. The powders were scattered randomly by releasing from a predefined height. The powder properties such as their centre Cartesian coordinates and radius were extracted from the DEM file and imported into the CFD model.

In the CFD model, the VOF method was used to capture the metal and gas phases. A Gaussian laser beam was modelled to scan across the powder bed. A single track was simulated to validate the geometries of the model with experimental results. The simulated melt pool geometries show close approximation with those from experiments. Next, a study on the formation of porosities was carried out. By varying the energy density on the powder bed, two types of porosities were observed. When low energy density parameters were used, there is insufficient energy to fully melt the powder within the laser beam. This resulted in gaps between the partially melted particles. There was also gaps between the substrate and powder which results in poor interlayer bonding and leads to delamination in printed parts. The second type of porosity observed was the keyhole porosity. When high energy density parameters were used, the keyhole generated due to recoil pressure was deep and unstable. In the model, the velocity vector of the molten metal was used to explain the collapse of the keyhole. When the keyhole collapsed, the gas trapped within the molten metal may not have sufficient time to escape before the metal solidifies and formed pores within

the melt track. These porosity are observed to be elliptical due to the effects of surface tension to minimize the surface area at the interface of the metal and gas.

Using the knowledge of the physics behind the single material model, a novel model for simulating multi-material in SLM was developed. In this thesis, two metals were simulated. A weight averaging method was introduced to determine the material properties of the melt pool and the effect of surface forces contributed by individual metals. A comparison between the melt pool geometries of experiment and simulation was done to validate the model. A study on the effect of interfacial surface tension between the liquid metals was conducted. Interfacial tensions of 0, 0.5 and 1 N m^{-1} were chosen to study the effects of increasing interfacial tensions. When metals have no interfacial tension, they are miscible and formed a homogenous mixture in the melt track. The surface of this melt track is smooth and similar to the shape of a single material melt track. When interfacial tension was introduced, there is a resultant force exerted on the surface molecules of the metals. This led to a liquid metal forming elliptical shape in the matrix of the other metal. When this occurred at the surface of the melt track, it gave rise to uneven surface. This can result in formation of defects due to the uneven distribution of powder on the subsequent layer. Due to the experimental measurement limitation, the values of interfacial tension between metals cannot be determined. By running simulations with different interfacial tension values and comparing them with the melt track from experiments, approximate values for interfacial tension can be obtained. However, there are limitations to the current model. It does not account for chemical reaction between metals which can produce a new phase such as intermetallic compounds.

6.2 Future works

Based on this thesis, there are several recommendations for future studies. Firstly, the limitation of the multi-material model was due to the lack of material information. The interfacial tension between the metals showed significant impact on the homogeneity within the melt track. For metals with interfacial tensions, it can lead to discontinuity in the melt track and cause defects. Future work can be performed to determine the interfacial tension between the metals for the model to predict the interactions between the metals accurately.

Secondly, the multi-material model did not include the chemical reactions and solubility between metals. There are metals that will form intermetallic compounds during the SLM process. These intermetallic compounds have different material properties than the original metals. The solubility of a metal in another metal will affect the resultant mechanical properties and has to be considered when simulating the two metals. Future work can incorporate the formation of these intermetallic compounds within the current model and the solubility between the metals.

Thirdly, this thesis explored the effects of constant interfacial tension between two liquid metals. It is unknown if the interfacial tension is temperature dependent or temperature gradient dependent due to the lack of research in this area. If the interfacial tension is dependent on temperature or temperature gradient, it can greatly alter the interactions of the molten metals. Future work can include the modelling of temperature dependent interfacial tension and temperature gradient dependent interfacial tension. Results of the simulation can be compared to experiment results for validations.

Lastly, current model uses materials with very similar properties. Future work can include using two metals with significant differences in their melting points, vaporizing temperatures, absorptivities, surface tensions. These properties will affect the surface forces experienced by the difference metals which will affect the melt track's geometry.

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