Microstructure modelling for metallic additive manufacturing: a review

Joel Heang Kuan Tan, Swee Leong Sing and Wai Yee Yeong
Singapore Centre for 3D Printing, School of Mechanical & Aerospace Engineering, Nanyang Technological University, Singapore

ABSTRACT
The microstructure of metals depends on the additive manufacturing (AM) process and the process parameters. However, experimentation on different process parameters for different materials is costly and time-consuming. To overcome these challenges, numerical simulations provide insights that allow prediction of microstructure formed under different process parameters. Microstructure modelling requires coupling of macro-scale thermal model or experimentally measured temperature profiles with either a meso-scale or micro-scale microstructure model. In this review, the commonly used AM techniques for metals are introduced, followed by a discussion on the microstructure of parts fabricated using these processes. This review then presents the latest models used in simulating different microstructural aspects of metal AM parts. In addition, the models were compared and the potential and challenges in microstructure modelling were discussed.

ARTICLE HISTORY
Received 27 June 2019
Accepted 4 October 2019

KEYWORDS
Additive manufacturing; simulation; microstructure; numerical model; 3d printing; powder bed fusion; directed energy deposition

1. Introduction
Additive manufacturing (AM) is a group of manufacturing methods that can produce highly customised parts catering to the low volume markets (Chua and Leong 2017). According to ISO/ASTM 52900:2017, AM is the general term for those technologies that create physical objects by successive addition of materials based on geometrical representations. AM involves the process of joining materials to make parts from 3D model data, usually layer upon layer, as opposed to subtractive manufacturing and formative manufacturing methodologies. AM is able to build complex geometries without the need for moulds which potentially reducing part count (Gibson, Rosen, and Stucker 2010; Atzeni and Salmi 2012). The aerospace and healthcare industries can use AM to their advantage with metals like stainless steel, titanium, cobalt chrome and nickel alloys (Vandenbroucke and Kruth 2007; Brunette et al. 2012; Cantor, Assender, and Grant 2015). While AM can achieve complex geometry, the manufacturing process is highly complex with numerous factors affecting the properties of the part. An important feature of metal is its microstructure. For a given metal, there can be a variety of microstructural features that affects its mechanical properties. The size of grains, microsegregation of alloying elements, phases within the metal and size of dendrites relates to the tensile strength and ductility (Warren and Boettinger 1995; Lu et al. 2010). During the AM process, the microstructure is formed in-situ and would therefore depend largely on the process parameters and material used. The process parameters are dependent on the metal AM method used.

1.1. Additive manufacturing methods for metals
There are two commonly used techniques in AM of metals, powder bed fusion (PBF) and directed energy deposition (DED). PBF process includes selective laser sintering (SLS), selective laser melting (SLM) and electron beam melting (EBM). SLM and EBM are used for the fabrication of metals.

Both processes start from digital files. 3D computer-aided design (CAD) files are sliced into layers and the data are then sent to the machine for printing. The next step is a set of cycles that melts the powders layer by layer until the final product is completed. In each cycle, a fixed thickness of powder is deposited onto a substrate and a heat source is applied to the powder in a raster scanning pattern. The heat source could either be laser or electron beam. This melts the layer of powder, bonding it to the substrate or to the previously melted layer. Lastly, the platform is lowered and the cycle repeats.

DED processes, on the other hand, can use wire or powder as the feedstock, and energy sources could use laser, electron beam and electricity. As DED machines can have 5 axis of movement, the layer added to the
CAD file may need to be sliced in a computer-aided manufacturing (CAM) software. Energy source and feedstock could be applied to the feedstock coaxially or off-axis. The feedstock fed as an energy source is applied to it. The feedstock material is melted and bonds with the substrate thereby forming a layer. Examples of SLM and coaxial laser direct energy powder deposition setups are shown in Figure 1.

While both PBF and DED processes build the part layer by layer, there can be distinct differences between the two. PBF machines are currently limited to build up layers in a single direction. DED machines can have 5+ axis systems allowing layers to be built in any direction provided there is no clashing of the part and tool head. This allows DED to repair parts in multiple directions while PBF is limited to repairing in a single direction. Parts produced by PBF can have better resolution due to the smaller powder size and smaller energy spot size as compared to DED machines.

1.2. Microstructure of additive manufactured metals

AM processes have been used to fabricate certain alloys like 316L stainless steel, Ti-6Al-4V and Inconel 625/718 which are common alloys used in marine and aerospace applications. The microstructure of metals determines the mechanical properties of the part such as yield strength, ductility and hardness (Peel et al. 2003; Ziętala et al. 2016; Guo et al. 2017; Shuai et al. 2018). Due to their wider applications, most of the modelling works done have been on these materials, however, they have the potential to be applied for new alloys. New alloys that have been processed by AM includes, but not limited to, Al–Cu alloys (Wang et al. 2018; Martinez, Todd, and Mumtaz 2019), Al–Cu–Mg (Nie et al. 2018), Al–Cu–Mg–Si (Wang et al. 2018), Al–Zn–Si–Mg–Cu (Casati et al. 2019), Cu–Sn alloys (Mao et al. 2018; Tan et al. 2019), Cu–10Zn (Zhang et al. 2019) and Cu–Cr (Uchida et al. 2019). AM process predominantly produces columnar grains with a mix of equiaxed grains that consist of cellular dendrites (Figure 2) (Murr et al. 2012; Frazier 2014; Roehling et al. 2017). The columnar grains typically grow along the build direction causing anisotropy and difference in performance with varying build orientations (Lewandowski and Seifi 2016). By varying the process parameters like the energy sources and feed types can lead to differences in grain structure (Frazier 2014). Ti-6Al-4V had columnar grains when printed with multiple tracks using electron beam-wire-DED and laser-powder-DED, however, when printed using laser-powder-DED for a single track the grains do not grow in a columnar fashion. The Ti-6Al-4V microstructure was finer in the electron beam-wire-DED as compared to the laser-powder-DED (Murr et al. 2012; Dehoff et al. 2015). Ti-6Al-4V was shown to exhibit near equiaxed prior-beta grains that quickly grow to large columnar grains after the initial layers, indicating that varying cooling rates and temperature gradient can induce changes in microstructure (Tan et al. 2015). The cooling rate and temperature gradient also affect dendritic formation. Cellular dendrites are formed when the cooling is fast, while slower cooling rates allow formation of secondary dendrite arm (Kou 2003). High cooling rate and low temperature gradient can cause an increase in mechanical properties, like in the case of Inconel 718 where the finer distributed laves phases are formed, leading to lesser chance of hot cracking (Nie, Ojo, and Li 2014). As the grain structure and dendrites affect the overall mechanical properties, it is important to know how different printing techniques and process parameters affects the grain structure.

![Figure 1. Schematic of selective laser melting and coaxial laser directed energy powder deposition.](image-url)
structure (Giffkins 1976; Baufeld, Van der Biest, and Gault 2010).

The microstructure of metals depends largely on the thermal gradient and cooling rate during solidification. By varying the process parameters, it is possible to alter the grain structure. Raghavan et al. used two different scanning strategies, one with line scans and another spot scanning. Line scans tend to cause columnar grains while spot scanning together with controlling the current, duration and distance between each spot lead to more equiaxed grains being formed (Raghavan et al. 2016). Dehoff et al. additionally alternate line and spot scanning within the same part to achieve different areas with columnar and equiaxed grains. The sequence in which the boundary area, equiaxed area and columnar area is printed first also matters as it affects the temperature gradient (Dehoff et al. 2015). In both cases, EBM is used and had the powder bed pre-heated to near melting temperature of the material, this which helps lower the overall temperature gradient allowing equiaxed grains to form.

It is shown that changing the parameters and scanning strategy can result in tailored microstructure (Körner et al. 2014; Parimi et al. 2014; Dehoff et al. 2015; Wei, Mazumder, and DebRoy 2015; Raghavan et al. 2016). Tailored microstructure can help in applications that require texture or the lack of it like in single crystal turbine blades and provide possibilities in grain boundary engineering.

Transition of columnar to equiaxed grains depends largely on the temperature gradient as well as the cooling rate. These values can be found experimentally or from computer simulations. Experimental methods can only investigate microstructure after the entire part is printed. In-situ monitoring of the AM process have limited capabilities and are restrained to monitor surface effects, and provide no information beyond the surface (Cléjsters et al. 2014; Huang et al. 2015; Everton et al. 2016; Lu and Wong 2018).

Computer simulations of the AM process help in understanding the evolution of temperature beyond the top surface. Simulations use the temperature results from thermal models to predict microstructure on varying length scales. As AM process involves building layer upon layer, the melt tracks experience multiple remelting. Experimental data can only give the grain structure after the entire build, while simulation provides access to the evolution of the grain structure throughout the process.

The aim of the paper is to review the different methods of microstructure modelling used specifically for AM metals. The different microstructure models are compared, and their strengths and limitations are explored.

## 2. Modelling for metal additive manufacturing

Modelling of microstructure requires coupling models at different length scales. First, a macro-scale thermal model is required to get the thermal history of the part during the AM process. The thermal model can come from simulation or from experimental data. Experimental data, however, would only capture the surface and a numerical model would be needed to translate it to a 3D melt pool. Simulation of the thermal model can range from a single melt track to multiple melt tracks and across multiple layers. Second, data from the thermal model is used as input to the microstructure model. Microstructure models can be further categorised based on another length scale, meso-scale and micro-scale. Meso-scale simulation refers to models that simulate multiple grains, while micro-scale simulation refers to models that simulate the dendritic formation.

### 2.1. Thermal modelling in additive manufacturing

Thermal numerical models can investigate the temperature the material would experience during the AM process. Thermal models can predict the temperature profile, fluid flow, porosity and be coupled to microstructure models or thermo-mechanical models to get the microstructure or residual stress and deformation (Vastola, Pei et al.; Denlinger, Heigel, and Michaleris 2015; Yang et al. 2018). The temperature profile could also be used to predict the amount of precipitate formed, columnar grain growth orientation and columnar to equiaxed transition (CET) (Liu et al. 2018; Yin et al. 2018; Kumara et al. 2019). Microstructure modelling uses thermal models to find the temperature history and shape of the scanned tracks as input. This section reviews the thermal models used in conjunction with microstructure models.

#### 2.1.1. Thermal models without fluid flow

Finite difference method (FDM) and finite element method (FEM) have been coupled with various microstructure models, typically simulating for large volumes of multiple tracks and layers (Mercelis and Kruth 2006; Zeng et al. 2015; Chen, Guillemot, and Gandin 2016; Zinovieva, Zinoviev, and Ploshikhin 2018). FEM/FDM solves for the heat equation partial differential equation (PDE):

$$\rho c_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = Q_s. \quad (1)$$

In Equation (1), $\rho$ is the density, $c_p$ is the specific heat.
capacity, $T$ is the temperature, $t$ is the time, $k$ is the thermal conductivity and $Q_s$ is the heat source added to the model. Heat loss by radiation and convection is sometimes added to the top surface as boundary conditions (Loh et al. 2015).

Simulating for PBF, FEM models often use elements of different materials. The top elements are assigned as the powder material and the remaining elements are the substrate material (Figure 3(a)). The powder element often has the density based on the porosity of the powder bed multiplied by the substrate density. The thermal conductivity is similarly dependent on the porosity of the powder bed (Chen, Guillemot, and Gandin 2016; Foroozmehr et al. 2016; Chiumenti et al. 2017). Elements that are assigned as powder material would change to substrate material once the temperature of the element goes above the liquidus temperature. Simulating for DED differs slightly from PBF models. Material has to be added while the heat source moves. FEM models do this by first placing dead/inactive elements above the substrate, as the heat source moves, the dead/inactive elements are set to be alive/active (Figure 3b) (Fallah et al. 2011). This simulates the material being fed and added to the melt.

| Simulation method | Phase field method | Modified cellular automata | Kinetic Monte Carlo | Cellular automata |
|-------------------|--------------------|---------------------------|---------------------|-------------------|
| Computational resource | High | High | Low | Moderate |
| Length scale | 0.025–0.2 µm | 0.3–0.4 µm | 1–10 µm | 1–10 µm |
| Mesh shape | Square | Square/hexagon | Points | Square/hexagon |
| Experiments required | Few, for validation | Few, for validation | Several, for tuning & validation | Few, for validation |
| Level of details | Dendrite shape | Dendrite shape | Grain size | Grain size |
| Probabilistic/Deterministic | √ Probabilistic | √ Deterministic | √ Probabilistic | √ Deterministic |
| Commercial software | Yes | No | No | No |
| Open source software | Yes | No | Yes | Limited |
| References | (Cao and Choi 2006; Fallah et al. 2012; Montiel et al. 2012; Sahoo and Chou 2014; Gong and Chou 2015; Sahoo and Chou 2016; Acharya, Sharon, and Staroselsky 2017; Keller et al. 2017; Kumara et al. 2019; Kumara et al. 2019) | (Wang, Lee, and Mclean 2003; Zhu, Lee, and Hong 2004; Michelic, Thuswaldner, and Bernhard 2012; Zaeem, Yin, and Felicelli 2013; Chen, Xu, and Liu 2014) | (Yang et al. 2000; Mishra and DebRoy 2004a; Mishra and DebRoy 2004b; Zhong 2011; Liu et al. 2014; Wang, Liu, and Wei 2014; Rodgers et al. 2016; Rodgers, Madison, and Tikare 2017; Wei, Elmer, and DebRoy 2017) | (Yin and Felicelli 2010; Zaeem, Yin, and Felicelli 2013; Wang et al. 2014; Rai, Markl, and Körner 2016; Zhou et al. 2016; Zinoviev et al. 2016; Dezfoli et al. 2017; Lopez-Botello et al. 2017; Panwisawas et al. 2017) |

Figure 2. Columnar grains observed in various additive manufactured metal alloys; (a) 316L stainless steel, (b) Ti6Al4V and (c) Inconel 625, ‘Comparison of microstructures and properties for a Ni-base superalloy (Alloy 625) fabricated by electron and laser beam melting’ by K. Amato et al. is licenced under CC BY 4.0 (Amato et al. 2012).
pool. Dead/inactive elements work by having its thermal conductivity set to near zero such that the temperature of the element would not change.

Meshing for FEM plays an important role in getting accurate temperature profiles and melt depths. Hexahedral element is commonly used as it provides better accuracy and works well with simple geometry used in simulations (Lindgren et al. 1997; Yin et al. 2018). AM processes have localised areas of large temperature changes in the area of the heat source. Chiumenti et al. suggested that in order to have better estimation of the temperature, the size of the element have to be smaller than the energy source spot size, Foroozmehr et al. used eight by eight elements within the laser spot (Foroozmehr et al. 2016; Chiumenti et al. 2017). Having high resolution throughout the entire mesh can lead to long computational time. As such, most models simulate a single melt track. In order to simulate a larger volume, Patil et al. used adaptive mesh refinement (AMR) to have higher resolution in and around the melt pool and progressively coarser mesh beyond the melt pool leading to a decrease in computing time by a hundred times (Patil et al. 2015). This allows solving for a larger area allowing investigations on scanning strategies involving simulating for multiple tracks. Denlinger used a similar method and found it to be 432 times faster than using static mesh (Denlinger 2018).

2.1.2. Thermal models with fluid flow in continuum scale or powder scale considering actual powder particles

Computational fluid dynamics (CFD) methods like the finite volume method (FVM) have been used to get the shape of the track, melt pool and the temperature history. FVM methods are used to solve the Navier-Stokes equation which can simulate effects like vaporisation and Marangoni effect seen in AM (Khairallah et al. 2016; Andani et al. 2017). This would lead to higher accuracies in the temperature distribution in the melt pool and also higher accuracies in geometry (Khairallah et al. 2016). In order to simulate the fluid flow within the melt, the mass and momentum equation have to be included alongside the energy equation (Gürtler et al. 2013; Yuan and Gu 2015):

\[
\frac{\delta}{\delta t}(\rho H) + \nabla \cdot (\rho \vec{v} H) - \nabla \cdot (k \nabla T) = Q_s, \quad (2)
\]

\[
\frac{\delta \rho}{\delta t} + \nabla \cdot (\rho \vec{v}) = M_s, \quad (3)
\]

\[
\frac{\delta \vec{v}}{\delta t} + \rho \vec{v} \cdot \nabla \vec{v} = -\nabla p + \mu \Delta \vec{v} + M_s \vec{v} + F. \quad (4)
\]

Equation (2) is the energy equation for heat conduction where \( H \) is the enthalpies and \( \vec{v} \) is the velocity of fluid. Equation (3) is the mass conservation equation where \( M_s \) is the mass source. In PBF where powders are already laid before simulating, the mass source can be considered as zero while in DED where powders are added while running would require the mass source term. Equation (4) is the momentum equation where \( \mu \) is the dynamic viscosity and \( F \) is a force term like gravitational force that may be included. The increase in the number of PDEs leads to an increase in computing power required. Most FVM models only simulate a single melt track in 3D (Fallah et al. 2012; Lee and Zhang 2015; Khairallah et al. 2016; Panwisawas et al. 2017). CFD of PBF can use varying types of powder distribution, either by powder...
packing density or using numerical models like discrete element method (DEM) (Lee and Zhang 2015; Zielinski et al. 2017). Numerical methods of packing powder led to irregular powder distribution that is closely resembling to actual powder deposition in PBF processes. CFD-DEM method has been used for DED processes as well, taking into account gas flow, powder flight and heating as well as interactions with the melt pool (Pinkerton 2015). The amount of details required of the simulation causes it to be even more computationally expensive as DEM is simulated together with CFD and gas flow has to be taken into account as well. While CFD can lead to more realistic tracks, literature of using CFD for DED processes is few.

The Lattice Boltzmann method (LBM) is another CFD method that is used to couple with microstructure models. LBM does not solve the Navier-Stokes equation, instead, it solves discrete Boltzmann equations to model the fluid flow (Rausch et al. 2017). LBM can simulate the powder distribution as well as the fluid flow and evaporation while FVM would require coupling with DEM to simulate the powder distribution (Khairallah et al. 2016; Liu and Wang 2017). LBM becomes comparatively more expensive when changing from 2D to 3D, with most 2D models being able to simulate multiple layers for a single track, a 3D model however, can simulate multiple tracks in a single layer (Körner, Bauereiß, and Attar 2013; Rai, Markl, and Körner 2016; Degenhardt 2017). LBM has been used to model PBF processes however no literature was found to have used LBM for DED processes at the time of writing.

CFD models have an average cell size of 5 µm and average domain of 150 × 1000 × 150 µm (Körner, Bauereiß, and Attar 2013; Lee and Zhang 2015; Zielinski et al. 2017). In comparison, FEM models have element size ranging from 25 µm to 5 mm and domain size ranging from 0.4 × 1 × 0.4 mm to 250 × 250 × 325 mm (Loh et al. 2015; Foroozemehr et al. 2016; Chiumenti et al. 2017). The model and element size can differ by three orders of magnitude. The number of cells for CFD also range in the millions while FEM elements tend to be less than a million. While CFD models can simulate multiple physical phenomena, the complexity and small cell size limit the total domain to be less than a millimetre in length, limiting the simulation to few short tracks. FEM models have many assumptions, reducing accuracy but increasing the size of the domain to accommodate multiple longer tracks and multiple layers.

2.2. Microstructure modelling in additive manufacturing

There are similarities between the melting of a single track in AM and welding. Welding typically adds material between two metal parts thereby joining them while AM adds material to a substrate or previously printed layer. The solidification of both welding and AM are very similar since both use a moving heat source to melt the added material leading to a moving melt pool. Since welding research is more developed, microstructure modelling techniques in welding can be applied and translated to AM (Seufzer 2014; Rolchigo et al. 2017).

There are three microstructure models that are reviewed, phase-field modelling (PFM), kinetic Monte Carlo (MC) and cellular automata (CA). CA and MC are considered meso-scale models as they simulate multiple grains mainly looking at the overall size and aspect ratio of the grains. PFM is considered a micro-scale model as it can simulate on the sub-grain level, getting the solute concentration, precipitates and dendrites shape. It also able to simulate multiple grains using multi-phase field models (Miyoshi et al. 2019).

The coupling between macro thermal model and the microstructure model can be done in two ways. The models can be weakly coupled, where the thermal model is simulated first and the thermal history is used as input to the microstructure model. Another way is to strongly couple them and simulate both at the same time, where information is shared and interacts between both models. Although strongly coupled simulations would be able to yield more accurate results, it requires longer computational time (Gandin et al. 1999). A schematic of the different microstructure models is shown in Figure 4 showing the boundary conditions and assumptions of the model.

2.2.1. Phase field modelling

PFM has been shown to be able to model solid, liquid and material phases within the same model. Microstructure evolution like grain coarsening and dendrite growth in forced convection could be simulated as well (Gránásy, Pusztai, and Warren 2004; Singer-Loginova and Singer 2008; Sahoo and Chou 2014). PFM is thermodynamically consistent, however, the interface width has to be thin in PFM increasing difficulty in modelling thereby limiting the size of the model (Elder et al. 2001). A large model with several interfaces will be too computationally expensive to run, especially if it is in 3D. While PFM provides the ability to simulate multiple phenomena with high accuracy, computational resources will be limiting factors (Francois et al. 2017).

2.2.1.1. Phase field modelling theory. PFM simulates microstructures by having all variables to be continuous across the interface. The interface can be a fraction of both solid and liquid. Mathematically, the description of the interface or otherwise called the phase field variable, \( \phi \), can be represented as \( \phi \in [-1, 1] \). During
the solidification process, the system of a fixed volume would tend towards a lower free energy in order to achieve stability (Boettinger et al. 2002; Kim and Kim 2005; Steinbach 2009):

\[ F = \int [f(\phi, c, T) + \omega g(\phi) + \varepsilon^2 |\nabla \phi|^2] dV, \quad (5) \]

where \( F \) is the total free energy of the system, \( f \) is the thermodynamic potential, \( c \) is the concentration, \( \omega g(\phi) \) is the double well potential, \( \varepsilon^2 |\nabla \phi|^2 \) is the phase-field gradient energy and \( V \) is the volume. The phase-field gradient energy is dependent on the gradient of the interface and therefore would be zero in fully solid and liquid regions. The thermodynamic potential is the sum of the free energies of the liquid and solid states. Over time, the system would decrease the total free energy of system. In order to solve the transient problem, the Allen-Cahn and Cahn–Hilliard equations can be used (Boettinger et al. 2002; Chen 2002; Kim and Kim 2005):

\[ \frac{\partial \phi}{\partial t} = -M_\phi \left[ \frac{\partial f}{\partial \phi} + \omega g'(\phi) - \varepsilon^2 \nabla^2 \phi \right], \quad (6) \]

\[ \frac{\partial c}{\partial t} = \nabla \cdot M_c \nabla \frac{\partial f}{\partial c}, \quad (7) \]

where \( M_\phi \) and \( M_c \) are the motilities of the phase field and concentration field at the interface respectively. In a multi-phase problem like in solidification of certain steels, there can be liquid, ferrite and austenite, each of these phases has its own variable, \( \phi_i(x, t) \) where \( i \) denotes the state that the field is. The sum of the phases in a multi-phase system has to reach unity,

\[ \sum_{i=1}^N \phi_i = 1 \quad (Boettinger et al. 2002). \]

2.2.1.2. Application of phase field modelling. Farzadi et al. used CFD and PFM to simulate the growth of columnar dendrites in the Al-Cu weld to investigate the solute concentration, dendrite arm spacing and undercooling at varying welding speed (Farzadi et al. 2008). The method used can be applied to the scanning of a single track in AM for binary alloys. Montiel et al. used...
2D PFM to investigate the CET of magnesium alloy during welding (Montiel et al. 2012).

FEM and PFM have been coupled to simulate AM processes. The temperature gradient and cooling rates were found using FEM and used as a boundary condition in PFM. Gong and Chou simulated in 2D for EBM of Ti-6Al-4V using FEM and PFM (Gong and Chou 2015). The thermal model shows that faster scanning speeds led to higher cooler, the cooling rate is used to find the distance between seeds for the PFM models too. The PFM model showed columnar prior-beta grains which grew faster with higher cooling rates and experimental results showed similar prior-beta grain sizes. However, the grain size was partially affected by the predetermined distance between seeds. Sahoo and Chou found the grain size differently, simulating from a single dendrite and using the primary dendrite arms spacing as the grain size (Sahoo and Chou 2016). Sahoo and Chou simulated the EBM process using a thermal model in 3D and a PFM model in 2D. A single dendrite was simulated and its primary dendrite arms grew in the columnar fashion and was compared to the experimental results showing columnar grains. The primary dendrite spacing and arm width were found to get smaller as scanning speed increases. The simulated dendrite arm spacing was larger than experimental results by approximately 0.5 µm. Within a melt pool, the solid–liquid interface can have different temperature gradient and solidification velocity at the bottom and trailing edge of the melt pool. Fallah et al. simulated for laser-powder-DED of Ti-Nb using 3D FEM to find the localised temperature gradient and solidification velocity which is input to 2D PFM models (Fallah et al. 2012). The thermal model found that the temperature gradient is smaller and the solidification velocity faster near the surface as compared to the bottom. PFM models for different temperature gradient and solidification velocity were simulated and the dendrite spacing was compared to experimental results. The PFM model was accurate except at the extreme ends where temperature gradient or solidification velocity is highest. Different PFM model or boundary conditions may need to be applied to get more accurate results. CFD can simulate the Marangoni flow which enhances cooling and thus can get more accurate melt pool shape and temperature profile. Acharya et al. simulated with SLM process for Inconel 718 using 2D PFM with the domain shaped like the melted track found using 3D CFD (Acharya, Sharon, and Staroselsky 2017). Although CFD was used, the PFM model had some differences with experimental results. The primary dendrite spacing and segregation of solutes tally with experimental results, however, the simulated results show secondary dendrites growing while experimental results show little to no secondary dendrites. These PFM models reduced the complexity by simplifying the alloys to binary alloys. However, PFM can also consider multi-phase and multi-components. Kumara et al. simulated with data from Thermo-Calc to incorporate multiple elements for Inconel 718. The model assumed a fixed cooling rate with no temperature gradient and simulated to study Laves phases during solidification and heat treatment (Kumara et al. 2019; Kumara et al. 2019).

2.2.2. Kinetic Monte Carlo
Kinetic MC modelling is a completely probabilistic simulation of the grain structure. MC is able to simulate grain structures over large volumes due to the low computational resource required. MC models differ from PFM models which simulate the solute concentration and dendrite shape, MC only models the grains therefore simulating on a different length scale. MC models provide the shape and size of grains.

2.2.2.1. Kinetic MC theory. The MC method is based on an atomistic simulation and the minimisation of the overall system energy. Each site on the lattice is given a number or orientation and if the neighbour of a site has a different orientation, it would add to the overall system energy. If the neighbour has the same orientation, there is no change in the system energy. Each site has a probability of changing orientation, if the change in orientation causes an increase, a random number would generate for that site and compare to an acceptance probability and if the random number is smaller than the acceptance probability, it is accepted. These are shown in the following (Yang et al. 2000; Rodgers, Madison, and Tikare 2017):

\[
\Delta E = J \sum [1 - \delta(l_j, l_k)],
\]

\[
P = \begin{cases} 
\exp \left( \frac{-\Delta E}{k_B T_0} \right), & \Delta E > 0, \\
1, & \Delta E \leq 0
\end{cases}
\]
recalculated and compared with the previous time step. In general, if the current step has an increase in overall energy, it is rejected and the previous time step configuration is kept. In order to simulate solidification, some modifications to the MC method have to be made. The grain boundary mobility is dependent on the temperature at the site and follows the Arrhenius equation (Yang et al. 2000; Rodgers, Madison, and Tikare 2017). Equation 9 is then modified to:

\[
P = \begin{cases} 
M_0 \exp \left( -\frac{Q_{\text{act}}}{R_g T} \right) \exp \left( -\frac{\Delta E}{k_B T_0} \right), & \Delta E > 0, \\
M_0 \exp \left( -\frac{Q_{\text{act}}}{R_g T} \right), & \Delta E \leq 0,
\end{cases}
\]

where \( M_0 \) is the Arrhenius pre-exponential factor, \( Q_{\text{act}} \) is the activation energy, \( R_g \) is the gas constant and \( T \) is the site temperature. MC method requires relatively lower computational resources and is able to simulate both 2D and 3D (Stefanescu 2015). It is able to simulate multiple laser passes and layers due to the low computation cost (Rodgers, Madison, and Tikare 2017).

2.2.2. Application of kinetic MC. MC methods have been used to simulate microstructure for casting, sintering and welding. It is also able to model the change of microstructure during recrystallisation and grain growth (Zhong 2011; Liu et al. 2014). Mishra and DebRoy used MC to predict grain sizes in the heat-affected zone (HAZ) due to solidification and grain growth in Ti6Al4 V during welding (Mishra and DebRoy 2004a; Mishra and DebRoy 2004b). The models showed potential to be used for simulating repairs using AM, especially to treated metal, which leads to HAZ. Thermal models are also coupled with MC to predict grain structures in welding (Yang et al. 2000; Wei, Elmer, and DebRoy 2017). Wei et al. capture the aspect ratio and grain sizes at varying welding speeds of aluminium alloys using CFD and MC. However, the model was not validated against experimental data (Wei, Elmer, and DebRoy 2017).

Rodgers et al. predicted the 3D microstructure in a single pass electron beam welding using MC and later increasing the number of scans extending it to EBM and electron beam powder DED (Rodgers et al. 2016; Rodgers, Madison, and Tikare 2017). The model was able to simulate a large volume capturing the crystal growth bias towards the scanning direction. While the model was able to capture the patterns of the experimental EBSD data, the aspect ratio and sizes are not fully captured. Sun et al. used different melt pool geometry in MC for the solidification of 316L and found equiaxed grains growing in the middle of the track for fast scanning speed (Sun et al. 2018). The results support experimental data that columnar grains being broken off each layer at faster scanning speed. However, the grain size and aspect ratio also differ from experimental data. While the MC method has been used extensively for welding, the use of it for AM is few. MC method, however, has the least computational cost and has the potential to model over large volumes.

2.2.3. Cellular automata

CA simulation is a probabilistic model with deterministic elements in it. The nucleation rate and dendrite direction are probabilistic while the growth of dendrites and preferential crystallographic direction is taken from theory. Similar to MC, CA simulates the grain structure rather than the dendrites. Having more equations to solve, CA uses more computational resources than MC but is able to capture grain angles and grow accordingly. This can lead to more accurate results.

2.2.3.1. Cellular automata theory. CA uses certain rules to change the state of a cell and in the case of solidification, the states are solid, liquid and mushy. CA requires a mesh of equally divided cells, usually square (2D) or cube shape (3D), with each cell interactive with its neighbouring cells by the rules. The CA model would require rules that govern the transition from solid to liquid, liquid to solid, setting of crystallographic orientation, speed and orientation of capturing neighbouring cells for crystal growth. CA follows the rules of solidification theory as well as some probability elements for nucleation. CA models are often coupled with macro thermal models to help in the rules of solid–liquid transition. CA models are like MC models in that both do not calculate the dendritic structures like secondary arm growth but instead simulate the grain structure allowing it to capture a larger scale. The changing of cell state from liquid to solid depends not only on temperature but the probability of nucleation as well. CA models use a probabilistic approach to determine nucleation, as undercooling, \( \Delta T \), drives the solidification, the continuous grain density, \( n \), is given by (Gandin and Rappaz 1994):

\[
n(\Delta T) = \int_0^{\Delta T} \frac{dn}{d(\Delta T)} d(\Delta T). \tag{11}
\]

A Gaussian distribution can be used to determine if a cell forms a nucleus:

\[
\frac{dn}{d(\Delta T)} = \frac{n_{\max}}{\sqrt{2\pi}} \exp \left[ -\frac{(\Delta T - \Delta T_{\text{mean}})^2}{2(\Delta T_{\sigma})^2} \right], \tag{12}
\]
where $n_{\text{max}}$ is the maximum nucleation density, $\Delta T$ is the undercooling of the liquid, $\Delta T_{\text{mean}}$ is the mean undercooling when nucleation occurs and $\Delta T_{n}$ is the standard deviation of the undercooling. Capturing of neighbouring cells by crystal growth is determined by solidification theory. One of the growth kinetics models is the Kurz-Giovanola-Trivedi (KGT) model. The KGT model assumes that the solid–liquid interface would grow at near absolute stability limit and the velocity can be found as a function of the undercooling (Kurz, Giovanola, and Trivedi 1986):

$$\Omega = \frac{C^* - C_0}{C^*(1 - K)} = IV\left\langle \frac{VR}{2D} \right\rangle,$$  \hspace{1cm} (13)

$$R = 2\pi \sqrt{\frac{\Gamma}{mg_c \xi_c - G}},$$  \hspace{1cm} (14)

$$\xi_c \approx \frac{\pi^2}{K \frac{VR^2}{2D}},$$  \hspace{1cm} (15)

$$\Delta T = mC_0 \left(1 - \frac{1}{\Omega(1 - K)} \right),$$  \hspace{1cm} (16)

where $\Omega$ is the solute supersaturation, $C^*$ is the liquid solute concentration at the tip of the dendrite, $C_0$ is the initial solute concentration, $D$ is the solute diffusion coefficient, $K$ is the partition coefficient, $R$ is the radius of the tip of the dendrite, $m$ is the slope of the liquidus, $\Gamma$ is the Gibbs-Thomson coefficient, $G_c$ is the solute gradient, $G$ is the thermal gradient and $\Delta T$ is the undercooling temperature. Solving equations 13–16 together would give a correlation between the undercooling temperature and the velocity of the dendrite growth.

2.2.3.2. Application of cellular automata. CA was developed for casting and has been adapted for welding and laser cladding (Rappaz and Gandin 1993; Zhan et al. 2008; Yin and Felicelli 2010; Wang et al. 2014). Wang et al. coupled FEM and CA models to predict the grain growth during a single pulse of the laser on Ti6Al4 V for laser cladding (Wang et al. 2014). The model captured the melt pool depth and grain structures for varying laser pulse duration. Dezfoli et al. used FEM and CA models to predict the effect of a secondary laser heat source on the microstructure (Dezfoli et al. 2017). The model was able to capture the difference in microstructure due to the varying melt pool dimension in 3D. The effects of secondary laser caused the thermal gradient and cooling rate which can cause grains to transit from columnar to equiaxed. Both models did not have the addition of materials that are required in AM but have shown the similarities and can be translated from welding to AM.

CA has been used to simulate the SLM process which was coupled with varying thermal macro models. Zinoviev et al. coupled FDM and CA to simulate SLM of 316L, getting the 2D grain structure at the traverse cross section of a melt track for multiple layers (Zinoviev et al. 2016). Although the model was able to capture the columnar growth, the experiment data displayed small amounts of equiaxed grains and some columnar grains being cut off by another columnar grain. This could be due to the model being only 2D and lack of nucleation that could happen in the experiment. Zinoviev et al. similarly coupled FDM and CA for 3D grains, however, the grains grew purely columnar which can be different from experimental data that had equiaxed grains (Zinovieva, Zinoviev, and Ploshikhin 2018). This leads to inaccurate grain structure as only columnar grains will grow from bottom to top since no nucleation occurs which differs from experimental data found. Koepf et al. simulated in 3D for multiple layers with multiple tracks per layer for EBM of Inconel 718 (Koepf et al. 2018). The thermal solution was found analytically and CA was used to simulate the grain structure and the simulated grain size and aspect ratio matched the experimental results well through the multiple layers. Similar to the models mentioned above, there are equiaxed grains mixed within the columnar grains which affects the overall grain structure to a certain extent. However, the cause for these equiaxed grains may not be fully understood and can be difficult to capture in the CA models. One issue that multiple tracks and layer CA models must deal with is the large memory required deal to the small cell sizes. Both CA and thermal models would require parallelisation and the thermal solution may need to be simplified. Koepf et al. used an analytical solution instead of a purely numerical simulation to reduce the computational resource. Koepf et al. used numerical simulation for the thermal model and reused the temperature profile at varying regions in the entire model, rotating by 90° at certain regions (Koepf et al. 2019). This reduced the computational memory and storage required for the entire thermal profile. Lopez-Botello et al. simulated the microstructure along the longitudinal cross section using 2D FEM and CA models for SLM of AA-2024 (Lopez-Botello et al. 2017). The model predicted columnar growth with grain sizes close to experiment data. Nucleation is captured based on experimental data with the probability of nucleation depending on the grain size. Although this method managed to capture the scattered grains, it requires experiments first for tuning of parameters. Rai et al. coupled CA with Lattice Boltzmann to find the microstructure of different laser scanning pattern (Rai, Markl, and Körner 2016). Although LBM is more accurate than FEM, it is...
computational resource heavy and difficult to translate to 3D. The grain sizes matched the experimental data that’s compared to other literature, however, the grain orientation could not be captured fully as it is simulated in 2D and cannot be compared to the EBSD results. Panwisawas et al. coupled CFD and CA models to predict the microstructure of Ti-6Al-4V using SLM (Panwisawas et al. 2017). While CFD provides greater detail in terms of melt pool shape and the flow in the melt is accounted for, the volume simulated is limited to a single scan track. This limits the study and single scan tracks may not be able to represent the overall grain structure.

CA has been modified to consider the momentum and species transport equations called modified cellular automata (MCA) (Zhu, Lee, and Hong 2004). MCA solves the additional equations by finite difference, which is an additional step CA does not have (Wang, Lee, and Mclean 2003). Unlike CA, MCA simulates on the micro-scale also getting the dendrite shape and solute concentration in a given melt pool that is solidifying. MCA has been shown to be able to model for multiple solute elements, CET and also include effects like convection in the melt pool (Zhu, Lee, and Hong 2004; Michelic, Thuswaldner, and Bernhard 2012; Chen, Xu, and Liu 2014). While having different equations and methods as PFM the results found were similar (Zaeem, Yin, and Felicelli 2013). However, MCA has not been applied to AM as of the time of writing.

2.3. Comparison of microstructure modelling methods

A comparison of the length scale and accuracy of the different models is shown in Figure 5. The smaller the length scale, the smaller the simulation time step needed, this to large amount of data created. Higher accuracy models tend to have more equations and variables to solve which requires more computational resources. In general, accurate models have small length scales, short time steps thus limiting the volume the model can simulate. CFD models tend to only simulate a single melt track while FEM models simulate multiple melt tracks. PFM models simulate a few dendrites while CA and MC models simulate the grain structure.

Comparing the models, PFM not only gives realistic dendrite shapes, but it also accounts for the solute distribution between the dendrite arms. When combined with thermodynamic databases, TTT and CTT curves, PFM can have not only very accurate details of solute distribution and dendrite shapes and sizes but also predict the composition of the various metals and intermetallic and transformation and growth of precipitates (Ferreira et al. 2017; Mullis, Bollada, and Jimack 2018; Böttger et al. 2019). All the PFM models for AM were in 2D and only simulated a few dendrites. This is most likely being due to the computational resources required thus making 3D models time-consuming and expensive to run. MCA has been modelled in 3D and have been shown to be more efficient and faster than PFM while having the similar results, however, simulations are also done on small number of dendrites (Wang, Lee, and Mclean 2003; Zaeem, Yin, and Felicelli 2013). In comparison, CA and MC were used to simulate multiple tracks and layers only capturing the grains thus only producing results like grain sizes, aspect ratio and CA grain angles. A comparison of all the models is shown in Table 1.

3. Potential and challenges of microstructure modelling in AM

3.1. Challenges

Modelling for microstructure requires thermal models as they provide the temperature, cooling rate and temperature gradient for inputs to the microstructure model. Having more accurate cooling rates and temperature gradients can lead to better predictability of microstructure. However, the length scale of the models is either a single track scan or multiple tracks and multiple layers, with CFD being used most often to simulate a single line and FEM for multiple tracks and layers. Most likely happens due to the computational resource limitation. FEM models have to use bulk material properties and the powder bed, the porosity of the powder bed is used to estimate the bulk properties. However, finding the porosity of the powder bed is difficult, the density of a powder bed can be estimated by the apparent density. The apparent density can be found using a Scott volumeter, but during the recoating of the powder during a PBF process the underlying surface is uneven and actual distribution of the powder is unknown, this will cause the density of the powder bed to vary. FEM models have codes developed to allow mesh refining and coarsening or having lumped heat per layer to reduce computational time and increase the volume simulated (Papadakis et al. 2014; Patil et al. 2015). However, the FEM codes were written to help improve simulation time for AM processes and commercial FEM software currently unable to reproduce it at the time of writing. CFD models, on the other hand, are not replicating the volume, FEM models are making but instead focus on the different phenomena in the melt pool. This leads to more accurate details which would be better for the microstructure model as better growth
kinetics can be predicted. A challenge thermal model face in getting accurate temperature is an accurate input of the heat source. FEM models tend to take a heat distribution either as a 2D input on the top surface or as a 3D volumetric heat (Loh et al. 2015; Yin et al. 2018). This heat input often uses estimated power and absorptivity. CFD models can use ray tracing to model laser PBF which leads to higher accuracy (King et al. 2015). However, in all models, the emissivity and absorptivity can change with temperature and this is difficult to capture in experiments.

Thermal models are considered macro scale in comparison with microstructure models which are micro- or meso-scale. MC and CA both are better suited to simulate large volumes as they require lesser calculations while PFM and MCA require more calculations and simulates a smaller volume. The choice of models comes down to the length scale required. Apart from the length scale, each microstructure models also face challenges.

Figure 5. Schematic diagram comparing different models in terms of length scale and accuracy; Representation of each models (a) Phase field Modelling, (b) Cellular automata, (c) kinetic Monte Carlo, ‘Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo’ by T. M. Rodgers et al. is licensed under CC BY 4.0 (Rodgers, Madison, and Tikare 2017), (d) Computational fluid dynamics, Solid Freeform Fabrication. Copyright 2015 The University of Texas at Austin. (Lee and Zhang 2015) and (e) Finite element method.

The dendrite shape and solute concentration that micro-scale models predict can be used to investigate new materials to be used in AM. Having an estimate on element phases and solute concentration can help in knowing if defects like hot cracking are likely to form or segregation of alloying elements (Keller et al. 2017; Gao et al. 2018). However, PFM and MCA also face certain challenges. Currently, both models only model the solidification portion without the melting portion. Instead, seeds are placed in predefined positions. While this may provide an estimate of the Primary dendrite arm spacing (PDAS), the actual size of the dendrite is dependent on the given spacing from each seed. This leads to bias based on the seed position placed and changing of material or process parameters may require changes in seed positioning or experiments to provide better positioning. Another challenge is the computational resources required in micro-scale modelling (Glicksman 2010). This limits the volume of the simulation within a single grain or a few grains.
Due to the nature of AM, depending on the scanning strategy, tracks can be re-melted several times. For PBF processes, tracks are often overlapping causing a single track to be melted at the sides and the next layer would also cause the top portion of the previous layer to melt. The grain structure of the metal would then depend on the melting and growing of grains from previously printed tracks. In order to track the grain structure, microstructure models would have to be able to simulate a large enough volume to investigate different scanning strategies. In this aspect meso-scale MC and CA models would work well as it has been shown to be able to model in 3D as well as multiple tracks and layers. A challenge for MC models is to get results closer to experimental data, although the trends of the grain structure are captured, the aspect ratio differs (Rodgers, Madison, and Tikare 2017; Sun et al. 2018). CA models face challenges in getting the scattered mix of equiaxed grains found in experimental data (Rai, Markl, and Körner 2016; Zinoviev et al. 2016; Zinovieva, Zinoviev, and Ploshikhin 2018). Most CA models depend on nucleation models used in casting or do not implement nucleation, similar to welding CA models. This leads to grains that grow indefinitely in the build direction which differs from experimental data. New nucleation methods may have to be used to capture nucleation in CA models.

Meshing plays an important role in numerical models and inappropriate meshing can lead to inaccurate results or alter results causing mesh anisotropy. PFM models have a very thin interface which requires very small cell sizes at the interface, however, the small cell size also reduces the time step of the model creating large amounts of data and requires more computational time for the same amount of time length (Zhang et al. 2019). Some models use adaptive meshing to reduce the number of total cells (Francois et al. 2017). Kinetic MC and CA also face a similar problem of having smaller cell sizes requiring small time steps leading to large amounts of data and computational resources. CA also can face mesh anisotropy and to counter this some models use hexagonal cells, however, majority of the models use the decentred square method developed by Gandin and Rappaz which allows square cells while eliminating mesh anisotropy (Gandin and Rappaz 1997; Dezfoli et al. 2017; Panwisawas et al. 2017).

### 3.2. Potentials

Most PFM models reviewed in this paper reduced the alloy to a binary alloy thus only finding the solute concentration or precipitate of a single solute. Microsegregation occurs in as-built AM parts and causes non-homogenous microstructure (Ghosh 2018). Simulating multicomponent alloy could help in studying how segregation occurs and possible workarounds, however, it would increase the computational time as the equations would have to solve the summations of each component (Nestler, Garcke, and Stinner 2005). MC models do not face this issue as it does not account for solutes. CA models use solidification theory which can account for multiple elements, however, most model also reduces it to binary or tertiary alloys (Zineviva, Columnar to equiaxed transition during alloy solidification).

While this paper reviews the microstructure modelling done for AM processes, the fundamental concepts can be also applied to post-processing heat treatments of AM parts as the thermal cycles also affect the microstructure despite the different heating and cooling rates. Numerous works have been done on post-process heat treatment of AM parts and how they affect the microstructure (Kajima et al. 2018; Kim et al. 2018; Kong et al. 2018; Kurzynowski et al. 2018; Salman et al. 2019). Using Inconel 718, Deng et al. applied heat treatment to the material produced by SLM, aiming to homogenise the microstructure and optimise the mechanical properties. While they observed that the heat treatments can precipitate the strengthening γ/γ′ phase, and dissolve the Laves phase and precipitate the δ phase depending on the heat treatment temperature, the mechanical properties are also improved due to the removal of residual stresses (Deng et al. 2018). Li et al. have similar observations, however, the anticorrosive ability of the material decreases after heat treatment (Li et al. 2019).

In this review, the focus is on the microstructural evolutions during the AM processes. The results from these models have the potential to be fed and linked to mechanical properties prediction of the AM parts. Recently, Ge et al. used an integrated modelling of process–structure–property relationship in laser AM for duplex titanium alloy. It is found that the formation of larger grain sizes and more α phase are due to higher scanning speed. This higher composition of α phase is then linked to higher mechanical properties (Ge et al. 2019). At current stage, most of the work done has linked the thermal simulations to the residual stresses in AM parts (Ding et al. 2011; Heigel, Michaleris, and Reutzel 2015; Yang et al. 2016; Zhao et al. 2017). The main challenge to link the different models together to achieve the microstructure to mechanical properties relation is the exchange of information between the individual model. Yan et al. have proposed to use a fixed format, flat-file database as a solution (Yan et al. 2018; Yan et al. 2018). However, more efficient approaches for information exchange have to be developed (Smith et al. 2016).
4. Conclusion

Numerical modelling can help in predicting microstructure without the need for experiments. The grain structure, microsegregation, precipitate and dendrite size can be predicted using varying microstructure models. In order to get it, two models are usually coupled together, thermal model and microstructure model. Two types of thermal models and three types of microstructure modelling for AM are reviewed. The macro thermal models predict the temperature, cooling rate and temperature gradient which are used as input for microstructure models.

Of the two types of thermal models, FEM is most often used model for multiple tracks and layers, while CFD is used for simulating limited number of tracks. FEM models ignore the flow of the fluid reducing the amount of computation required and thus are able to simulate a larger volume. CFD models often focus on the physics of the melt pool, requiring more computation resources. FEM models being able to simulate larger volumes can be used in microstructure modelling to simulate the grain structure where grains often grow over multiple layers. CFD models have more accurate cooling rate and temperature gradient which can be used to get more accurate microstructure.

There are two different scales that microstructure modelling can take place: micro-scale and meso-scale. Micro-scale models simulate the dendrites and the solute composition while meso-scale simulates the grain structures. PFM and MCA are able to simulate the micro-scale getting the segregation of alloying elements and finding the PDAS which relates to the local strength and hardness. It, however, requires large computational resource limiting its volume to simulate a few dendrites. MC and CA are able to simulate a larger volume getting the grain structure. The grain size and aspect ratio which relates to the strength and ductility of the part is found in both models. MC models, however, have poorer predictions in grain size as compared to CA models. PFM and MCA can be useful in finding how new materials would form in the AM process and can facilitate the addition of new materials for AM. The overall mechanical properties would also depend on the size and aspect ratio of grain structure which would require MC or CA to model. Depending on the type of mechanical properties to be predicted, simulation has to be done on different length scales.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

This research is supported by the National Research Foundation, Prime Minister’s Office, Singapore under its Medium-Sized Centre funding scheme.

Notes on contributors

Joel Heang Kuan Tan is a research student at the Singapore Centre for 3D Printing. He received his B.Eng. (Hons) in Mechanical Engineering from Nanyang Technological University, Singapore. His research interest is in additive manufacturing of metals, using simulation to relate and predict process parameters to resulting microstructure and mechanical properties.

Dr Swee Leong Sing is a Research Fellow at the Singapore Centre for 3D Printing. He received his B.Eng. (Hons) in Aerospace Engineering and Ph.D. in Mechanical Engineering from the Nanyang Technological University, Singapore. His research interest is in additive manufacturing for biomedical applications, focusing on materials creation and development, qualification and certification of additive manufactured medical devices. His doctoral thesis focuses on laser-based powder bed fusion processing of a novel titanium alloy for medical applications. Based on Web of Science (Clarivate Analytics), he has co-authored 28 peer-reviewed articles in the field of additive manufacturing or 3D printing. He currently has a H-index of 15 and is also the co-inventors for two patents on the powder bed fusion process.

Associate Professor Wai Yee Yeong received her B.Eng. (Hons) and Ph.D. in Mechanical and Aerospace Engineering from the Nanyang Technological University (NTU), Singapore. Prior to joining NTU as a faculty member in 2013, she has worked in the manufacturing industry at supervisory functions in research and development, with key focus in medical device industry. She is now serving as Associate Chair (Students) in the school. Her portfolio also includes serving as Programme Director (Aerospace and Defence) at Singapore Centre for 3D Printing (SC3DP), Deputy Director (Technical) for HP-NTU Digital Manufacturing Corporate Lab, and Co-Director of NTU Institute for Health Technologies. Her main research interest is in 3D printing, bioprinting and the translational of the advanced technologies for industrial applications. Her current research topics include 3D printing of new materials, hybrid electronic-mechanical structures and bioprinting for tissue engineering. She has co-authored 2 textbooks (published by World Scientific and Elsevier, respectively), published more than 130 peer-reviewed technical papers, with a current H-index of 29. To-date, she has filed 2 PCT patents in new alloy and new bioink formulations, and 2 Singapore provisional patents on 3D printing.

ORCID

Joel Heang Kuan Tan http://orcid.org/0000-0002-8357-1575
Swee Leong Sing http://orcid.org/0000-0002-3980-6605
Wai Yee Yeong http://orcid.org/0000-0003-3640-0877

References

Acharya, R., J. A. Sharon, and A. Staroselsky. 2017. “Prediction of Microstructure in Laser Powder bed Fusion Process.” Acta Materialia 124: 360–371.
Amato, K., J. Hernandez, L. Murr, E. Martinez, S. Gaytan, P. Shindo, and S. Collins. 2012. “Comparison of Microstructures and Properties for a Ni-Base Superalloy (Alloy 625) Fabricated by Electron and Laser Beam Melting.” *Journal of Materials Science Research* 1 (2): 3.

Andani, M. T., R. Dehghani, M. R. Karamooz-Ravari, R. Mirzaeifar, and J. Ni. 2017. “A Study on the Effect of Energy Input on Spatter Particles Creation During Selective Laser Melting Process.” *Additive Manufacturing* 20, 33–43.

Atzeni, E., and A. Salmi. 2012. “Economics of Additive Manufacturing for End-usable Metal Parts.” *The International Journal of Advanced Manufacturing Technology* 62 (9): 1147–1155.

Baufeld, B., O. Van der Biest, and R. Gault. 2010. “Additive Manufacturing of Ti-6Al-4V Components by Shaped Metal Deposition: Microstructure and Mechanical Properties.” *Materials & Design* 32 (1): 163–194.

Böttger, B., M. Apel, B. Daniels, L. Dankl, T. Göhler, and T. Jokisch. 2019. “Systematic Phase-field Study on Microstructure Formation During Brazing of Mar-M247 with a Si-Based AMS4782 Filler.” *Metallurgical and Materials Transactions A* 50 (4): 1732–1747.

Brunette, D. M., P. Tengvall, M. Textor, and P. Thomsen. 2012. *Titantium in Medicine: Material Science, Surface Science, Engineering, Biological Responses and Medical Applications*. New York: Springer Science & Business Media.

Cantor, B., H. Assender, and P. Grant. 2015. *Aerospace Materials*. Boca Raton: CRC Press.

Chen, L.-Q. 2002. “Phase-field Models for Microstructure Evolution.” *Annual Review of Materials Research* 32 (1): 113–140.

Chen, S., G. Guilletot, and C.-A. Gandin. 2016. “Three-dimen- sional Cellular Automaton-Finite Element Modelling of Solidification Grain Structures for Arc-welding Processes.” *Acta Materialia* 115: 448–467.

Chen, R., Q. Xu, and B. Liu. 2014. “A Modified Cellular Automaton Model for the Quantitative Prediction of Equiaxed and Columnar Dendritic Growth.” *Journal of Materials Science & Technology* 30 (12): 1311–1320.

Chiumenti, M., E. Neiva, E. Salsi, M. Cervera, J. Moya, Z. Chen, C. Lee, and C. Davies. 2017. “Numerical Modelling and Experimental Validation in Selective Laser Melting.” *Additive Manufacturing* 18: 171–185.

Chua, C. K., and K. F. Leong. 2017. “3D Printing and Additive Manufacturing – Principles and Applications.” World Scientific Publishing Co. Pvt. Ltd.

Clijsters, S., T. Craeghs, S. Buls, K. Kempen, and J. P. Kruth. 2014. “In Situ Quality Control of the Selective Laser Melting Process Using a High-Speed, Real-time Melt Pool Monitoring System.” *International Journal of Advanced Manufacturing Technology* 75 (5–8): 1089–1101.

Degenhardt, R. 2017. “Advanced Lattice Boltzmann Models for the Simulation of Additive Manufacturing Processes.” PhD Thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany.

Dehoff, R., M. Kirka, W. Sames, H. Bilheux, A. Tremsin, L. Lowe, and S. Babu. 2015. “Site Specific Control of Crystallographic Grain Orientation Through Electron Beam Additive Manufacturing.” *Materials Science and Technology* 31 (8): 931–938.

Deng, D., R. L. Peng, H. Brodin, and J. Moverare. 2018. “Microstructure and Mechanical Properties of Inconel 718 Produced by Selective Laser Melting: Sample Orientation Dependence and Effects of Post Heat Treatments.” *Materials Science and Engineering: A* 713: 294–306.

Denlinger, E. R. 2018. “Development and Numerical Verification of a Dynamic Adaptive Mesh Coarsening Strategy for Simulating Laser Power Bed Fusion Processes.” In *Thermo-Mechanical Modeling of Additive Manufacturing*, 199–213. Butterworth-Heinemann.

Denlinger, E. R., J. C. Heigel, and P. Michaleris. 2015. “Residual Stress and Distortion Modeling of Electron Beam Direct Manufacturing Ti-6Al-4V.” Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture 229 (10): 1803–1813.

Dexfoil, A. R. A., W.-S. Hwang, W.-C. Huang, and T.-W. Tsai. 2017. “Determination and Controlling of Grain Structure of Metals After Laser Incidence: Theoretical Approach.” *Scientific Reports* 7: 41527.

Ding, J., P. Colegrove, J. Mehnens, S. Ganguly, P. M. Sequeira Almeida, F. Wang, and S. Williams. 2011. “Thermo-mechanical Analysis of Wire and Arc Additive Layer Manufacturing Process on Large Multi-Layer Parts.” *Computational Materials Science* 50 (12): 3315–3322.

Ding, J., P. Colegrove, J. Mehnens, S. Ganguly, P. M. Sequeira Almeida, F. Wang, and S. Williams. 2011. “Thermo-mechanical Analysis of Wire and Arc Additive Layer Manufacturing Process on Large Multi-Layer Parts.” *Computational Materials Science* 50 (12): 3315–3322.

Dzefzol, A. R. A., W.-S. Hwang, W.-C. Huang, and T.-W. Tsai. 2017. “Determination and Controlling of Grain Structure of Metals After Laser Incidence: Theoretical Approach.” *Scientific Reports* 7: 41527.

Elder, K., M. Grant, N. Provatnas, and J. Kosterlitz. 2001. “Sharp Interface Limits of Phase-Field Models.” *Physical Review E* 64 (2): 021604.

Everton, S. K., M. Hirsch, P. Stravroulakis, R. K. Leach, and A. T. Clare. 2016. “Review of In-situ Process Monitoring and in-Situ Metrology for Metal Additive Manufacturing.” *Materials & Design* 95: 431–445.

Fallah, V., M. Alimardani, S. F. Corbin, and A. Khajepour. 2011. “Temporal Development of Melt-pool Morphology and Clad Geometry in Laser Powder Deposition.” *Computational Materials Science* 50 (7): 2124–2134.

Fallah, V., M. Amoorezaei, N. Provatnas, S. Corbin, and A. Khajepour. 2012. “Phase-field Simulation of Solidification Morphology in Laser Powder Deposition of Ti–Nb Alloys.” *Acta Materialia* 60 (4): 1633–1646.

Farzadi, A., M. Do-Quang, S. Serajzadeh, A. Kokabi, and G. Amberg. 2008. “Phase-field Simulation of Weld Solidification Microstructure in an Al–Cu Alloy.” *Modelling and Simulation in Materials Science and Engineering* 16 (6): 065005.

Ferreira, A. F., K. G. Paradela, P. Felipe Junior, Z. Alcântara Júnior, and A. Garcia. 2017. “Phase-Field Simulation of Microsegregation and Dendritic Growth During Solidification of Hypoeutectic Al–Cu Alloys.” *Materials Research* 20 (2): 423–429.

Foroozmehr, A., M. Badrossamay, E. Foroozmehr, and S. Golabi. 2016. “Finite Element Simulation of Selective Laser Melting Process Considering Optical Penetration Depth of Laser in Powder Bed.” *Materials & Design* 89: 255–263.

Francois, M. M., A. Sun, W. E. King, N. J. Henson, D. Tourret, C. A. Bronkhorst, N. N. Carlson, C. K. Newman, T. Haut, and J.
Bakosi. 2017. "Modeling of Additive Manufacturing Processes for Metals: Challenges and Opportunities." Current Opinion in Solid State and Materials Science. Accessed 18 October 2019. https://wwwosti.gov/servlets/purl/1344361.

Frazier, W. E. 2014. “Metal Additive Manufacturing: a Review.” Journal of Materials Engineering and Performance 23 (6): 1917–1928.

Gandin, C.-A., J.-L. Desbiolles, M. Rappaz, and P. Thevoz. 1999. “A Three-Dimensional Cellular Automation-Finite Element Model for the Prediction of Solidification Grain Structures.” Metallurgical and Materials Transactions A 30 (12): 3153–3165.

Gandin, C.-A., and M. Rappaz. 1994. “A Coupled Finite Element-Cellular Automaton Model for the Prediction of Dendritic Grain Structures in Solidification Processes.” Acta Metallurgica et Materialia 42 (7): 2233–2246.

Ge, P., Z. Zhang, Z. J. Tan, C. P. Hu, G. Z. Zhao, and X. Guo. 2019. “An Integrated Modeling of Process-Structure-Property Relationship in Laser Additive Manufacturing of Duplex Titanium Alloy.” International Journal of Thermal Sciences 140: 329–343.

Ghosh, S. 2018. “Predictive Modeling of Solidification During Laser Additive Manufacturing of Nickel Superalloys: Recent Developments, Future Directions.” Materials Research Express 5 (1): 012001.

Gibson, I., D. W. Rosen, and B. Stucker. 2010. Additive Manufacturing Technologies. New York: Springer.

Giffins, R. C. 1976. “Grain-boundary Sliding and Its Accommodation During Creep and Superplasticity.” Metallurgical and Materials Transactions A 7 (8): 1225–1232.

Glickman, M. E. 2010. Principles of Solidification: an Introduction to Modern Casting and Crystal Growth Concepts New York: Springer Science & Business Media.

Gong, X., and K. Chou. 2015. “Phase-field Modeling of Microstructure Evolution in Electron Beam Additive Manufacturing." JOM Journal of the Minerals Metals and Materials Society 67 (5): 1176–1182.

Gránásy, L., T. Pusztai, and J. A. Warren. 2004. “Modelling Polycrystalline Solidification Using Phase Field Theory.” Journal of Physics: Condensed Matter 16 (41): R1205.

Guo, P., B. Zou, C. Huang, and H. Gao. 2017. “Study on Microstructure, Mechanical Properties and Machinability of Efficiently Additive Manufactured AISI 316L Stainless Steel by High-Power Direct Laser Deposition.” Journal of Materials Processing Technology 240: 12–22.

Gürtler, F., M. Karg, K. Leitz, and M. Schmidt. 2013. “Simulation of Laser Beam Melting of Steel Powders Using the Three-Dimensional Volume of Fluid Method.” Physics Procedia 41 (1): 874–879.

Heigel, J. C., P. Michaleris, and E. W. Reutzel. 2015. “Thermo-mechanical Model Development and Validation of Directed Energy Deposition Additive Manufacturing of Ti–6Al–4V.” Additive Manufacturing 5: 9–19.

Huang, Y., M. C. Leu, J. Mazumder, and A. Donmez. 2015. “Additive Manufacturing: Current State, Future Potential, Gaps and Needs, and Recommendations.” Journal of Manufacturing Science and Engineering 137 (1): 014001.

Kajima, Y., A. Takaichi, N. Kitiikundecha, T. Nakamoto, T. Kimura, N. Nomura, A. Kawasaki, T. Hanawa, H. Takahashi, and N. Wakabayashi. 2018. “Effect of Heat-Treatment Temperature on Microstructures and Mechanical Properties of Co–Cr–Mo Alloys Fabricated by Selective Laser Melting.” Materials Science and Engineering: A 726: 21–31.

Keller, T., G. Lindwall, S. Ghosh, L. Ma, B. M. Lane, F. Zhang, U. R. Kattner, E. A. Lass, J. C. Heigel, and Y. Idell. 2017. “Application of Finite Element, Phase-Field, and Calphad-Based Methods to Additive Manufacturing of Ni-Based Superalloys.” Acta Materialia 139: 244–253.

Khairallah, S., A. T. Anderson, A. Rubenchik, and W. E. King. 2016. “Laser Powder-bed Fusion Additive Manufacturing: Physics of Complex Melt Flow and Formation Mechanisms of Pores, Spatter, and Denudation Zones.” Acta Materialia 108: 36–45.

Kim, S. G., and W. T. Kim. 2005. “Phase-Field Modeling of Solidification.” Journal of Crystal Growth 261 (1): 135–158.

Kim, Y.-K., S.-H. Park, J.-H. Yu, B. AIMangour, and K.-A. Lee. 2018. “Improvement in the High-Temperature Creep Properties via Heat Treatment of Ti-6Al-4V Alloy Manufactured by Selective Laser Melting.” Materials Science and Engineering: A 715: 33–40.

King, W. E., A. T. Anderson, R. Ferencz, N. Hodge, C. Kamath, S. A. Khairallah, and A. M. Rubenchik. 2015. “Laser Powder Bed Fusion Additive Manufacturing of Metals; Physics, Computational, and Materials Challenges.” Applied Physics Reviews 2 (4): 041304.

Koepf, J. A., M. R. Gotterbarm, M. Markl, and C. Körner. 2018. “3D Multi-Layer Grain Structure Simulation of Powder Bed Fusion Additive Manufacturing.” Acta Materialia 152: 119–126.

Koepf, J., D. Soldner, M. Ramsperger, J. Mergheim, M. Markl, and C. Körner. 2019. “Numerical Microstructure Prediction by a Coupled Finite Element Cellular Automaton Model for Selective Electron Beam Melting.” Computational Materials Science 162: 148–155.

Kong, D., X. Ni, C. Dong, L. Zhang, C. Man, J. Yao, K. Xiao, and X. Li. 2018. “Heat Treatment Effect on the Microstructure and Corrosion Behavior of 316L Stainless Steel Fabricated by Selective Laser Melting for Proton Exchange Membrane Fuel Cells.” Electrochimica Acta 276: 293–303.

Kou, S. 2003. Welding Metallurgy. Hoboken, NJ: John Wiley.

Körner, C., A. Bauereiß, and E. Attar. 2013. “Fundamental Consolidation Mechanisms During Selective Beam Melting of Powders.” Modelling and Simulation in Materials Science and Engineering 21 (8): 085011.

Körner, C., H. Helmer, A. Bauereiß, and R. F. Singer. 2014. “Tailoring the Grain Structure of IN718 During Selective Electron Beam Melting.” MATEC Web of Conferences, EDP Sciences.

Kumara, C., D. Deng, F. Hanning, M. Raanes, J. Moverare, and P. Nylén. 2019. “Predicting the Microstructural Evolution of Electron Beam Melting of Alloy 718 with Phase-Field Modeling.” Metallurgical and Materials Transactions A 50 (5): 2527–2537.

Kumara, C., A. Segerstark, F. Hanning, N. Dixit, S. Joshi, J. Moverare, and P. Nylén. 2019. “Microstructure Modelling of...
Laser Metal Powder Directed Energy Deposition of Alloy 718. *Additive Manufacturing* 25: 357–364.

Kurz, W., B. Giovanola, and R. Trivedi. 1986. “Theory of Microstructural Development During Rapid Solidification.” *Acta Metallurgica* 34 (5): 823–830.

Kurzynowski, T., K. Gruber, W. Stopyra, B. Kuznich, and E. Chlebus. 2018. “Correlation Between Process Parameters, Microstructure and Properties of 316L Stainless Steel Processed by Selective Laser Melting.” *Materials Science and Engineering: A* 718: 64–73.

Lee, Y., and W. Zhang. 2015. “Mesoscopic Simulation of Heat Transfer and Fluid Flow in Laser Powder bed Additive Manufacturing.” *Proceedings of the Annual International solid Freeform fabrication Symposium, Austin, TX, USA.*

Lewandowski, J. J., and M. Seif. 2016. “Metal Additive Manufacturing: A Review of Mechanical Properties.” *Annual Review of Materials Research* 46: 151–186.

Li, J., Z. Zhao, P. Bai, H. Qu, B. Liu, L. Li, L. Wu, R. Guan, H. Liu, and Z. Guo. 2019. “Microstructural Evolution and Mechanical Properties of IN718 Alloy Fabricated by Selective Laser Melting Following Different Heat Treatments.” *Journal of Alloys and Compounds* 772: 861–870.

Lindgren, L.-E., H.-A. Häggblad, J. McDill, and A. S. Oddy. 1997. “Automatic Remeshing for Three-Dimensional Finite Element Simulation of Welding.” *Computer Methods in Applied Mechanics and Engineering* 147 (3-4): 401–409.

Liu, Y., L. Cheng, Q. Zeng, Z. Feng, J. Zhang, J. Peng, C. Xie, and K. Guan. 2014. “Monte Carlo Simulation of Polycrystalline Microstructures and Finite Element Stress Analysis.” *Materials & Design* 55: 740–746.

Liu, D., and Y. Wang. 2017. “Mesoscale Multi-Physics Simulation of Solidification in Selective Laser Melting Process Using a Phase Field and Thermal Lattice Boltzmann Model.” *ASME 2017 International design engineering Technical Conferences and Computers and information in engineering Conference, American Society of mechanical Engineers, Cleveland, Ohio.*

Liu, S., H. Zhu, G. Peng, J. Yin, and X. Zeng. 2018. “Microstructure Prediction of Selective Laser Melting AISi10Mg Using Finite Element Analysis.” *Materials & Design* 142: 319–328.

Loh, L.-E., C.-K. Chua, W.-Y. Yeong, J. Song, M. Mapar, S.-L. Sing, Z.-H. Liu, and D.-Q. Zhang. 2015. “Numerical Investigation and an Effective Modelling on the Selective Laser Melting (SLM) Process with Aluminium Alloy 6061.” *International Journal of Heat and Mass Transfer* 80: 288–300.

Lopez-Botello, O., U. Martinez-Hernandez, J. Ramirez, C. Pinna, and K. Mumtaz. 2017. “Two-dimensional Simulation of Grain Structure Growth Within Selective Laser Melted AA-2024.” *Materials & Design* 113: 369–376.

Lu, J., K. Luo, Y. Zhang, G. Sun, Y. Gu, J. Zhou, X. Ren, X. Zhang, L. Zhang, and K. Chen. 2010. “Grain Refinement Mechanism of Multiple Laser Shock Processing Impacts on ANSI 304 Stainless Steel.” *Acta Materialia* 58 (16): 5354–5362.

Lu, Q. Y., and C. H. Wong. 2018. “Aditive Manufacturing Process Monitoring and Control by non-Destructive Testing Techniques: Challenges and in-Process Monitoring.” *Virtual and Physical Prototyping* 13 (2): 39–48.

Mao, Z., D. Z. Zhang, J. Jiang, G. Fu, and P. Zhang. 2018. “Processing Optimisation, Mechanical Properties and Microstructural Evolution During Selective Laser Melting of Cu-15Sn High-tin Bronze.” *Materials Science and Engineering: A* 721: 125–134.

Martinez, R., I. Todd, and K. Mumtaz. 2019. “In Situ Alloying of Elemental Al-Cu12 Feedstock Using Selective Laser Melting.” *Virtual and Physical Prototyping* 14 (3): 242–252.

Mercells, P., and J.-P. Kruth. 2006. “Residual Stresses in Selective Laser Sintering and Selective Laser Melting.” *Rapid Prototyping Journal* 12 (5): 254–265.

Michel, S., J. Thusswaldner, and C. Bernhard. 2012. “A Modified Cellular Automaton Method for Polydimensional Modelling of Dendritic Growth and Microsegregation in Multicomponent Alloys.” *IOP Conference Series: Materials Science and engineering, IOP Publishing.*

Mishra, S., and T. DebRoy. 2004a. “Grain Topology in Ti–6Al–4V Welds – Monte Carlo Simulation and Experiments.” *Journal of Physics D: Applied Physics* 37 (15): 2191.

Mishra, S., and T. DebRoy. 2004b. “Measurements and Monte Carlo Simulation of Grain Growth in the Heat-Affected Zone of Ti–6Al–4V Welds.” *Acta Materialia* 52 (5): 1183–1192.

Miyoshi, E., T. Takaki, M. Ohno, Y. Shibuta, S. Sakane, and T. Aoki. 2019. “Large-scale Phase-Field Simulation of Three-Dimensional Isothermal Grain Growth in Polycrystalline Thin Films.” *Modelling and simulation in Materials Science and Engineering* 27 (5): 054003.

Montiel, D., L. Liu, L. Xiao, Y. Zhou, and N. Provatas. 2012. “Microstructure Analysis of AZ31 Magnesium Alloy Welds Using Phase-Field Models.” *Acta Materialia* 60 (16): 5925–5932.

Mullis, A. M., P. C. Bollada, and P. K. Jimack. 2018. “Phase-Field Modelling of Intermetallic Solidification.” *TMS Annual Meeting & Exhibition, Springer, Phoenix.*

Murr, L. E., S. M. Gaytan, D. A. Ramirez, J. Hernandez, K. N. Amato, P. W. Shindo, F. R. Medina, and R. B. Wicker. 2012. “Metal Fabrication by Additive Manufacturing Using Laser and Electron Beam Melting Technologies.” *Journal of Materials Science & Technology* 28 (1): 1–14.

Nestler, B., H. Garcke, and B. Stinner. 2005. “Multicomponent Alloy Solidification: Phase-Field Modeling and Simulations.” *Physical Review E* 71 (4): 041609.

Nie, P., O. Ojo, and Z. Li. 2014. “Numerical Modeling of Microstructure Evolution During Laser Additive Manufacturing of a Nickel-Based Superalloy.” *Acta Materialia* 77: 85–95.

Nie, X., H. Zhang, H. Zhu, Z. Hu, L. Ke, and X. Zeng. 2018. “Analysis of Processing Parameters and Characteristics of Selective Laser Melted High Strength Al-Cu-Mg Alloys: From Single Tracks to Cubic Samples.” *Journal of Materials Processing Technology* 256: 69–77.

Panwisawas, C., C. Qiu, M. J. Anderson, Y. Sovani, R. P. Turner, M. M. Attallah, J. W. Brooks, and H. C. Basoalto. 2017. “Mesoscale Modelling of Selective Laser Melting: Thermal Fluid Dynamics and Microstructural Evolution.” *Computational Materials Science* 126: 479–490.

Papadakis, L., A. Loizou, J. Risse, S. Bremen, and J. Schrage. 2014. “A Computational Reduction Model for Appraising Structural Effects in Selective Laser Melting Manufacturing: a Methodical Model Reduction Proposed for Time-Efficient Finite Element Analysis of Larger Components in Selective Laser Melting.” *Virtual and Physical Prototyping* 9 (1): 17–25.

Parimi, L. L., G. Ravi, D. Clark, and M. M. Attallah. 2014. “Microstructural and Texture Development in Direct Laser Fabricated IN718.” *Materials Characterization* 89: 102–111.

Patil, N., D. Pal, H. K. Rafi, K. Zeng, A. Moreland, A. Hicks, D. Beeler, and B. Stucker. 2015. “A Generalized Feed Forward
Dynamic Adaptive Mesh Refinement and Derefinement Finite Element Framework for Metal Laser Sintering—Part I: Formulation and Algorithm Development.” Journal of Manufacturing Science and Engineering 137 (4): 041001.

Peel, M., A. Steuwer, M. Preuss, and P. Withers. 2003. “Microstructure, Mechanical Properties and Residual Stresses as a Function of Welding Speed in Aluminium AA5083 Friction Stir Welds.” Acta Materialia 51 (16): 4791–4801.

Pinkerton, A. J. 2015. “Advances in the Modeling of Laser Direct Metal Deposition.” Journal of Laser Applications 27 (51): S15001.

Raghavan, N., R. Dehoff, S. Pannala, S. Simunovic, M. Kirka, J. Turner, N. Carlson, and S. S. Babu. 2016. “Numerical Modeling of Heat-Transfer and the Influence of Process Parameters on Tailoring the Grain Morphology of IN718 in Electron Beam Additive Manufacturing.” Acta Materialia 112: 303–314.

Rai, A., M. Markl, and C. Körner. 2016. “A Coupled Cellular Automaton–Lattice Boltzmann Model for Grain Structure Simulation During Additive Manufacturing.” Computational Materials Science 124: 37–48.

Rappaz, M., and C.-A. Gandin. 1993. “Probabilistic Modelling of Microstructure Formation in Solidification Processes.” Acta Metallurgica et Materialia 41 (2): 345–360.

Rausch, A. M., V. E. Küng, C. Pobel, M. Markl, and C. Körner. 2017. “Predictive Simulation of Process Windows for Powder Bed Fusion Additive Manufacturing: Influence of the Powder Bulk Density.” Materials 10 (10): 1117.

Rodgers, T. M., J. D. Madison, and V. Tikare. 2017. “Simulation of Metal Additive Manufacturing Microstructures Using Kinetic Monte Carlo.” Computational Materials Science 135: 78–89.

Rodgers, T. M., J. D. Madison, V. Tikare, and M. C. Maguire. 2016. “Predicting Mesoscale Microstructural Evolution in Electron Beam Welding.” JOM Journal of the Minerals Metals and Materials Society 68 (5): 1419–1426.

Roehling, T. T., S. S. Wu, S. A. Khairallah, J. D. Roehling, S. S. Soezeri, M. F. Crumb, and M. J. Matthews. 2017. “Modulating Laser Intensity Profile Ellipticity for Microstructural Control During Metal Additive Manufacturing.” Acta Materialia 128: 197–206.

Rolchigo, M. R., M. Y. Mendoza, P. Samimi, D. A. Brice, B. Martin, P. C. Collins, and R. LeSar. 2017. “Modeling of Ti-W Solidification Microstructures Under Additive Manufacturing Conditions.” Metallurgical and Materials Transactions A 48 (7): 3606–3622.

Sahoo, S., and K. Chou. 2014. “Review on Phase-Field Modeling of Microstructure Evolutions: Application to Electron Beam Additive Manufacturing.” ASME 2014 International Manufacturing Science and Engineering Conference, MSEC 2014 collocated with the JSME 2014 International Conference on Materials and Processing and the 42nd North American Manufacturing Research Conference.

Sahoo, S., and K. Chou. 2016. “Phase-field Simulation of Microstructure Evolution of Ti–6Al–4 V in Electron Beam Additive Manufacturing Process.” Additive Manufacturing 9: 14–24.

Salman, O. O., C. Gammer, A. K. Chaubey, J. Eckert, and S. Scudino. 2019. “Effect of Heat Treatment on Microstructure and Mechanical Properties of 316L Steel Synthesized by Selective Laser Melting.” Materials Science and Engineering: A 748: 205–212.

Seufzer, W. J. 2014. “Additive Manufacturing Modeling and Simulation: A Literature Review for Electron Beam Free Form Fabrication.” Accessed 18 October 2019. https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20140005339.pdf.

Shuai, C., L. Xue, C. Gao, Y. Yang, S. Peng, and Y. Zhang. 2018. “Selective Laser Melting of Zn–Ag Alloys for Bone Repair: Microstructure, Mechanical Properties and Degradation Behaviour.” Virtual and Physical Prototyping 13 (3): 146–154.

Singer-Loginova, I., and H. Singer. 2008. “The Phase Field Technique for Modeling Multiphase Materials.” Reports on Progress in Physics 71 (10): 106501.

Smith, J., W. Xiong, W. Yan, S. Lin, P. Cheng, O. L. Kafka, G. J. Wagner, J. Cao, and W. K. Liu. 2016. “Linking Process, Structure, Property, and Performance for Metal-Based Additive Manufacturing: Computational Approaches with Experimental Support.” Computational Mechanics 57 (4): 583–610.

Stefanescu, D. 2015. Science and Engineering of Casting Solidification. New York: Springer.

Steinbach, I. 2009. “Phase-field Models in Materials Science.” Modelling and Simulation in Materials Science and Engineering 17 (7): 073001.

Sun, Z., X. Tan, S. B. Tor, and C. K. Chua. 2018. “Simultaneously Enhanced Strength and Ductility for 3D-Printed Stainless Steel 316L by Selective Laser Melting.” NPG Asia Materials 10 (4): 127.

Tan, X., Y. Kok, Y. J. Tan, M. Descoins, D. Mangelinck, S. B. Tor, K. F. Leong, and C. K. Chua. 2015. “Graded Microstructure and Mechanical Properties of Additive Manufactured Ti–6Al–4 V via Electron Beam Melting.” Acta Materialia 97: 1–16.

Tan, Z., X. Zhang, Z. Zhou, Z. Hou, Y. Yang, X. Guo, Z. Wang, X. Wu, G. Wang, and D. He. 2019. “Thermal Effect on the Microstructure of the Lattice Structure Cu-105n Alloy Fabricated Through Selective Laser Melting.” Journal of Alloys and Compounds 787: 903–908.

Uchida, S., T. Kimura, T. Nakamoto, T. Ozaki, T. Miki, M. Takemura, Y. Oka, and R. Tsubota. 2019. “Microstructures and Electrical and Mechanical Properties of Cu-Cr Alloys Fabricated by Selective Laser Melting.” Materials & Design 175: 107815.

Vandenbroucke, B., and J.-P. Kruth. 2007. “Selective Laser Melting of Biocompatible Metals for Rapid Manufacturing of Medical Parts.” Rapid Prototyping Journal 13 (4): 196–203.

Vastola, G., Q. X. Pei, and Y. W. Zhang. Predictive Model for Porosity in Powder-bed Fusion Additive Manufacturing at High Beam Energy Regime.” Additive Manufacturing 22: 817–822.

Wang, P., L. Deng, K. G. Prashanth, S. Pauly, J. Eckert, and S. Scudino. 2018. “Microstructure and Mechanical Properties of Al-Cu Alloys Fabricated by Selective Laser Melting of Powder Mixtures.” Journal of Alloys and Compounds 735: 2263–2266.

Wang, P., C. Grammer, F. Brenne, K. G. Prashanth, R. G. Mendes, M. H. Rummeli, T. Gemming, J. Eckert, and S. Scudino. 2018. “Microstructure and Mechanical Properties of a Heat-Treatable Al-3.5Cu-1.5Mg-1Si Alloy Produced by Selective Laser Melting.” Materials Science and Engineering: A 711: 562–570.

Wang, W., P. D. Lee, and M. Mclean. 2003. “A Model of Solidification Microstructures in Nickel-Based Superalloys: Predicting Primary Dendrite Spacing Selection.” Acta Materialia 51 (10): 2971–2987.
Wang, R., Y. Liu, and D. Q. Wei. 2014. “Microstructures in Solidification Simulation of Electron Beam Scanning with MC in Molten Pool. Advanced Materials Research.” In *Advanced Materials Research*, Vol. 898, 168–172. Trans Tech Publications.

Wang, Z.-J., S. Luo, H.-W. Song, W.-D. Deng, and W.-Y. Li. 2014. “Simulation of Microstructure During Laser Rapid Forming Solidification Based on Cellular Automaton.” *Mathematical Problems in Engineering* 2014. doi:10.1155/2014/627528.

Warren, J. A., and W. J. Boettinger. 1995. “Prediction of Dendritic Growth and Microsegregation Patterns in a Binary Alloy Using the Phase-Field Method.” *Acta Metallurgica et Materialia* 43 (2): 689–703.

Wei, H., J. Elmer, and T. DebRoy. 2017. “Three-dimensional Modeling of Grain Structure Evolution During Welding of an Aluminum Alloy.” *Acta Materialia* 126: 413–425.

Wei, H., J. Mazumder, and T. DebRoy. 2015. “Evolution of Solidification Texture During Additive Manufacturing.” *Scientific Reports* 5: 16446.

Zhan, X., Z. Dong, Y. Wei, and Y. Xu. 2008. “Dendritic Grain Growth Simulation in Weld Molten Pool Based on CA-FD Model.” *Crystal Research and Technology* 43 (3): 253–259.

Zhang, J., X. Li, D. Xu, and R. Yang. 2019. “Recent Progress in the Simulation of Microstructure Evolution in Titanium Alloys.” *Progress in Natural Science: Materials International* 29 (3): 295–304.

Zhang, S., H. Zhu, Z. Hu, X. Zeng, and F. Zhong. 2019. “Selective Laser Melting of Cu10Zn Alloy Powder Using High Laser Power.” *Powder Technology* 342: 613–620.

Zielinski, J., S. Vervoort, H.-W. Mindt, and M. Megahed. 2017. “Numerical Modeling of the Thermal Behavior and Residual Stress in the Direct Metal Laser Sintering Process of Titanium Alloy Products.” *Additive Manufacturing* 14: 126–136.

Zhou, X., H. Zhang, G. Wang, X. Bai, Y. Fu, and J. Zhao. 2016. “Simulation of Microstructure Evolution During Hybrid Deposition and Micro-Rolling Process.” *Journal of Materials Science* 51 (14): 6735–6749.

Zhu, M., S. Lee, and C. Hong. 2004. “Modified Cellular Automaton Model for the Prediction of Dendritic Growth with Melt Convection.” *Physical Review E* 69 (6): 061610.

Zielinski, J., S. Vervoort, H.-W. Mindt, and M. Megahed. 2017. “Influence of Powder bed Characteristics on Material Quality in Additive Manufacturing.” *BHM Berg-und Hüttenmännische Monatshefte* 162 (5): 192–198.

Ziętala, M., T. Durejko, M. Polański, I. Kunce, T. Płociński, W. Zieliński, M. Łazińska, W. Stępiowski, T. Czujko, and K. J. Kurzydlowski. 2016. “The Microstructure, Mechanical Properties and Corrosion Resistance of 316 L Stainless Steel Fabricated Using Laser Engineered Net Shaping.” *Materials Science and Engineering: A* 677: 1–10.

Zinoviev, A., O. Zinovieva, V. Ploshikhin, V. Romanova, and R. Balokhonov. 2016. “Evolution of Grain Structure During Laser Additive Manufacturing. Simulation by a Cellular Automata Method.” *Materials & Design* 106: 321–329.

Zinovieva, O., A. Zinoviev, and V. Ploshikhin. 2018. “Three-dimensional Modeling of the Microstructure Evolution During Metal Additive Manufacturing.” *Computational Materials Science* 141: 207–220.