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REVIEW OF MICROSCALE AND MESOSCALE SIMULATION OF LASER POWDER BED FUSION

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Abstract. Additive manufacturing (AM) is an advanced method of manufacturing complex parts layer by layer until the required design is achieved. Laser powder bed fusion (L-PBF) is used to produce parts with high resolution because of low layer thickness. L-PBF is based on laser beam and material interaction where the powder material is melted and then solidified. This occurs in a short time frame of the order of 0.02 seconds and makes the whole process challenging to be studied in real time. Studies have shown the development of numerical methods and the use of simulation software to understand the laser beam and material interaction. This phenomenon is key to understanding the material behavior under melting and mechanical properties of the part produced by L-PBF process as it is directly linked with the solidification of the melted powder material. A detailed study of the laser beam and material interaction is needed on a microscale and mesoscale level as it provides a better understanding and helps in the development of the given material for the L-PBF process. This review provides a comprehensive understanding of the background for the use of simulation in AM and the different simulation scales of feature under interest.

The main conclusion from this review is the need to develop a methodology to use simulation at micro and mesoscale level to understand the laser beam and material interaction and improve the efficiency of the L-PBF process using this data.

1 INTRODUCTION

Additive manufacturing (AM) is a manufacturing technique that allows freedom in design as parts are manufactured layer by layer [1]. Among the different AM processes, laser-based powder bed fusion (L-PBF) has demonstrated the highest resolution for producing complex parts using metals since the layers are very thin, around 0.04 mm [2]. L-PBF involves melting and solidification of metal powder by laser beam [1]. This process is challenging as it has many different parameters affecting it [3].

The different parameters affecting interaction between laser beam and material within the L-PBF process are: material parameters, process parameters and equipment parameters [4]. Material parameters are related to the powder material used for manufacturing and process parameters are related to the setting up the laser and powder material for the interaction phenomenon. Equipment parameters are related to the L-PBF machine which is used for manufacturing. Table 1 is a list of the different parameters concerning the L-PBF process.

Table 1. Parameters affecting L-PBF process

Parameter types	List of parameters	References
Material	Packing density, Particle size distribution, Powder layer thickness; Etc.	[5]
Process	Laser power, Powder spreading speed, Scan speed; Etc.	[6]
Equipment	Gas flow, Build volume, Recoater design; Etc.	[7]

Table 1 consists of the list of different parameters namely material, process and equipment related. Figure 1 describes interaction between laser beam and material, and this is an important part of the L-PBF process. [8]

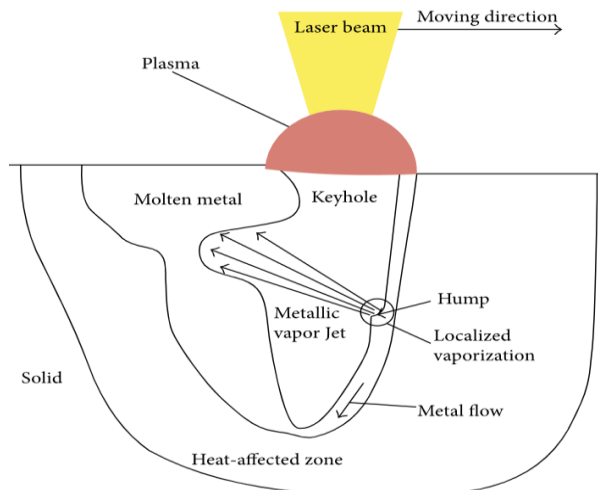


Figure 1. Laser beam and material interaction [8].

As it can be observed from figure 1, the laser beam melts the metal powder which forms melt pool. As melt pool moves with laser beam, molten metal solidifies to form solid metal along the path travelled by the laser beam [8]

The interaction between laser beam and metal material happens fast, as beam moves at c. 1000 m/s and this is where the formation of the melt pool happens [9]. The diameter of laser beam is only ca. 0.1 mm, and melt pool formed is slightly larger than that [10]. The quality of the process and the parts produced depends heavily on this phase of the process. This has been established in the research

of Hofmeister et al. where characteristics of melt pool like size and cooling rate determine the initial microstructure and material properties for a given material [11].

Figure 2 shows input and output parameters of the L-PBF process from the point of view of the raw material, the melt pool and AM part.

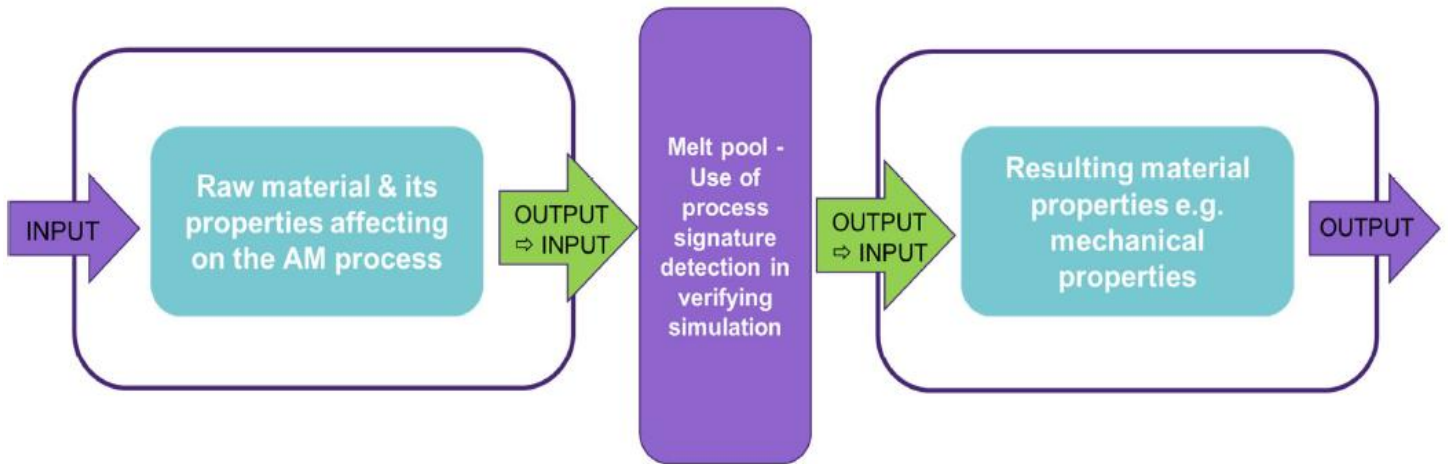


Figure 2. Input and output parameters in L-PBF when raw material, L-PBF process itself and AM part are considered.

As it can be seen from figure 2, the first building block of the L-PBF process is the raw material, which is metal powder. This is followed by the melt pool which forms upon the interaction of laser beam with powder material. In situ process signal detection is used at this stage of the L-PBF process which involves setting up equipment like high speed cameras, thermal imaging devices etc. to gather data in real time. The last building (see figure 2) block is the manufactured parts and their mechanical properties.

Sun et al. defined the parameters describing melt pool as the melt pool size, temperature, temperature gradient, melt lifetime, melt pool dimensions, melt pool viscosity, melt pool stability etc. for an L-PBF process [12]. Formation of the melt pool, its movement and its solidification are challenging to study in real time, as the process occurs and lasts for a short time span of around 0.01 seconds [13]. It is also important to understand the effect of material parameters in L-PBF process, since the incident laser beam heat source is directly applied on the top powder layer of the scanned region, it is critical to consider the material parameters as the melt pool begins to form here [14]. By the use of simulation, Cheng et al. (2021) have found out that the melt pool must have an optimum depth for optimum heat conduction and solidification. This was concluded by creating different laser scan tracks and studying the effect of laser parameters like energy density and scanning speed on the melt pool. The experimental results showed the melt pool depth was higher for high energy density and lower scan speed. [15]. Wischeropp et al. (2019) studied the packing density and powder layer height of Ti6Al4V and SS 17 4-PH by using simulation and then verifying the results experimentally. In this study, topography measurements and simulation were conducted for the powder beds of the two different materials for different process parameters such as powder spreading speed. The true

powder layer height was measured as a verification method for the simulation conducted and it was concluded that the height of the molten powder layer was equal to the levelling height of the build platform in both experimental and simulation results [16].

2 AIM AND PURPOSE OF THIS STUDY

The research [14]–[16] on the topic of simulation of the melt pool parameters, laser and material parameters, powder behaviour etc. sets the precedent for the use of simulation for studying the interaction between laser beam and metal material which shapes the L-PBF process. The objective of this study is to present the real-life application of simulation in the L-PBF process from different perspectives such as scale of feature, type of simulation and also the different software used by researchers. The aim of this study is to become the basis to approach the study of melt pool formation via different approaches using simulation.

Another objective here is to understand the laser beam and material interaction of the L-PBF process via the concept of simulation. Simulation enables the study of various phenomena occurring during the laser beam material interaction without the use of experimental setup. This saves time, cost and speeds up the process development for L-PBF. This is an ideal scenario for an industry which will enable cost cutting and save manpower. Simulation can also be applied in material development for L-PBF process which equally benefits researchers in the academic area and also in the industry.

Figure 3 presents how many publications are done in 2010-2022 in field of simulation when different scale of simulation is considered.

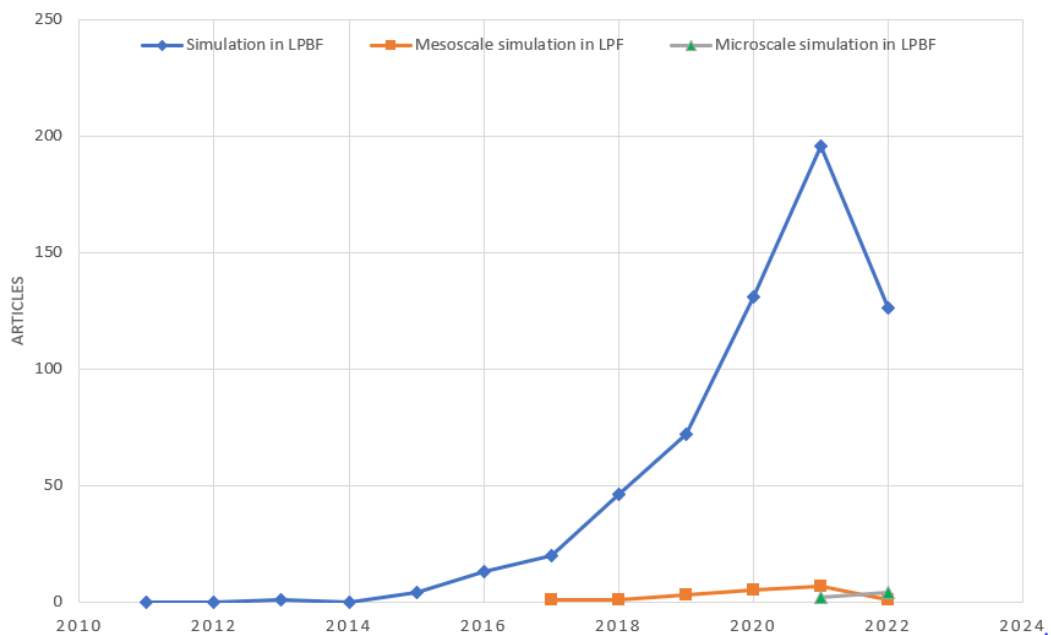


Figure 3. Articles published on simulations in L-PBF in 2010-2022

As it can be seen from the figure 3, research in simulation in L-PBF in the last decade is on an upward trend in terms of the articles published, A clear gap can be noticed in the research between the simulation in L-PBF and the simulation in L-PBF at micro and mesoscale level.

This has been identified as the gap area in the scope of this study on the basis of the data extracted from the Scopus database. This article will review the micro and mesoscale simulation method and their application to study the L-PBF process.

3 SIMULATION IN L-PBF

3.1 Use of simulation in L-PBF process

Simulation in L-PBF can mean a number of things. In the scope of this study, simulation in L-PBF will mean the simulation concerned with meso and microscale level as the focus is on the laser beam and material interaction. The meso and microscale levels is of the order of tens of microns(μm), which is the size of the powder particles that is used as a raw material for the L-PBF process [17]. Researchers have developed numerical models based on the thermal and mechanical aspects of L-PBF process for understanding laser beam and material interaction. These models have also been used to study the melt pool characteristics as a function of the thermal history of the L-PBF process [18][19]. Bayat et al. has listed the various physical phenomena occurring during the laser beam and material interaction as evaporation, melting, solidification, thermal radiation, laser absorption, liquid metal flow, recoil pressure etc. It was established in this research that melt pool of L-PBF can be studied as a function of these phenomena. In-situ process signal detection of these physical phenomena in L-PBF in real time includes the use of complicated setup and processing large amounts of data which is seen in the work of Bugatti et al. Hence, researchers [20][21] adopted the concept of thermal and mechanical based simulation to study the phenomena occurring during the laser beam and material interaction.

The time frame in which the laser beam and material interaction occurs is of the order of 0.01 seconds and the speed at which the laser beam moves is ca. 1000 mm/s. Studying the melt pool characteristics in this short time frame is challenging and hence numerical models like thermo-mechanical models have been suggested according to this research [22]. The research of Song et al. encourages that the use simulation in L-PBF removes the prospect of trial error methodology to develop the L-PBF process[23]. This establishes a strong background for the use of simulation in L-PBF process.

The scale at which simulation in L-PBF is often performed is at macroscale level or part scale level, to estimate the mechanical properties of the fabricated components in real time conditions [24][25]. While macroscale simulation continues to dominate the aspect of simulation in L-PBF, figure 4 indicates different length scales at which simulation is performed in L-PBF. It has been concluded in the research of Liu et al. and Wang et al. that control over the L-PBF process at these scales allows for control over the microstructure[26]. Wang et al. have taken a multi-track scan approach to understand the evolution of titanium alloy powder on a microscale level. The motivation behind choosing multi track approach was to understand the repeatability nature of the simulation. This study concluded that simulating multiple tracks of printing in conduction mode not only results in the formation of a long columnar microstructure, but also allows for the control in formation of it. This finding alone shows the importance of studying the L-PBF process at these scale levels.

Simulation at mesoscale and microscale is the key to understanding the laser beam and material interaction in L-PBF process [27]. Mesoscale simulation of L-PBF has been used in various studies to understand the behavior of metal powder after the laser beam interacts with

it [28]–[30]. This has been closely studied in the research of Lee et al. where a single linear track of melt pool formation for stainless steel 316 grade has been simulated. This study concluded that melt pool surface profile largely depended on the size of the powder particles and the packing density of the powder bed. The powder particles studied were of the order of 40 μm which is on a mesoscale level and an individual mesh size of the order of 3 μm was used in this model to solve the continuum conservation equations related to the powder particles.

Microscale simulation in L-PBF is used to understand the formation of the microstructure of the parts being manufactured. By controlling the formation of the microstructure, the mechanical properties like hardness, strength and toughness can be controlled as well [31]. The microscale simulation model is often paired with a macroscale thermal simulation model, as seen in the research of Pei et al. [32]. It was concluded from this approach that the thermal history and solidification phenomenon of the L-PBF process is key to understand the microstructure of the printed parts. Figure 4 provides a summary of the various phenomena in L-PBF that are associated with mesoscale and microscale level [33].

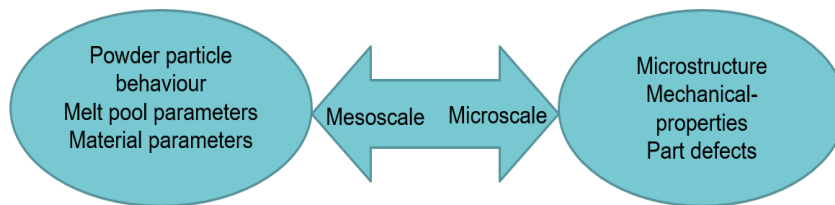


Figure 4. Phenomena in L-PBF concerning scales of interest

As it can be seen from figure 4, the mesoscale is associated with powder particle behavior within L-PBF as the powder particles used in L-PBF are of the order of ca. 50 μm . This scale can be used to study the melt pool characteristics from the point of view of the powder material [34]. The research performed by Chen et al. applied mesoscale simulation coupled with thermo-mechanical model to understand the melt pool surface profile as a function of powder morphology [35]. It was concluded that the morphology of powder particles played a key role in the formation of melt pool surface after interaction of the laser beam with the powder [36]. Microscale in L-PBF is often associated with microstructure characteristics of the parts being printed [37]. Studies performed by Babu et al. have combined microscale models with thermal models to study the formation of microstructure. The researchers used the thermal history from the laser beam and material interaction simulation model and developed the phase field model for simulating microstructure [38]. They have concluded that the part properties like tensile strength, hardness and ductility are dependent on the different phases formed during microstructure evolution.

3.2 Methods used to simulate the laser beam and material interaction- micro and mesoscale

The simulation of the laser beam and material interaction in L-PBF consists of developing a thermo-mechanical model containing a powder substrate and a heat source, as seen across different studies [39][40], [41]. A thermo-mechanical model was defined in the research of Heigl et al. as a model created to analyze the thermal and mechanical phenomena occurring in a given process[42]. In L-PBF, heat source is the laser beam which interacts with the powder substrate. Powder substrate is defined in the research of Chen et al. as the layer of the powder

that is spread on the build plate where the powder is melted and solidified to form a component according to the required design. The method used to carry out powder substrate modelling in this research is DEM (Discrete Element method). The powder bed in L-PBF consists of a large number of powder particles which are differentiated by size, morphology, packing etc. The research explains the motivation behind choosing DEM as a suitable method when dealing with granular particles. It is due to the ability of DEM to include the effect of material properties, size distribution and morphology on the simulation which is conducted [43].

The simulation of melting of the powder and melt pool formation is performed by different methods such as Finite Element Method (FEM), Finite Volume Method (FVM) and a combination of DEM-FVM/FEM [44]. FEM and FVM are defined as mathematical methods which are applied within certain boundaries in a given volume. The formation of the melt pool is driven by capillary forces and the Marangoni effect [45], which means that fluid dynamics concerning the melt pool and heat transfer phenomena come into play. The melt pool consists of molten metal, plume, spatter etc. The temperature gradient of the melt pool is really high as the solidification happens in the order of 0.2 seconds. This supports the use of FVM or FEM, which is used to solve the complex equations governing these phenomena, as the melt pool is assumed as a confined space with a given amount of volume. The use of DEM-FVM method to simulate the melt pool formation is supported by the different studies of Xia et al. and Wang et al. as FVM was used in this research to analyze melt pool characteristics such as surface tension and velocity, in correlation with laser parameters such as hatch spacing and laser power[46]. It was concluded that the use of FVM...

After the formation of the melt pool, Solidification of molten metal drives the formation of the microstructure of the component being manufactured since the shape and size of the grains in the microstructure depends on the solidification behavior [47]. The mechanical properties of the material such as hardness, tensile strength, toughness, ductility etc. are influenced by the grain sizes and shapes within the microstructure[47]. To simulate the solidification phenomenon and predict the microstructure, phase field (PF) model can be utilized. This model solves the problems related to solidification dynamics, thereby predicting the microstructure of the material [48]. PF model is used by combining the thermal data of the L-PBF process with the PF simulation which predicts the microstructure by estimating the grain boundaries and grain shapes.

Table 2 summarizes the methods of simulation used in the process of powder spreading and powder melting in L-PBF process.

Table 2. Applications of simulation approaches [49]

Simulation approach	Application area	Physical phenomenon	L-PBF phenomena
Finite Volume method (FVM)	Powder melting	Thermal fluid behavior	Melt pool behaviour
Finite Element method (FEM)	Powder melting	Thermal fluid behavior	Melt pool behaviour
Discrete Element method (DEM)	Powder spreading	Particle dynamics	Powder bed behaviour

DEM-FVM and DEM-FEM	Powder melting	Particle dynamics and Thermal fluid behavior	Powder bed and melt pool behaviour
Phase Field (PF)	Melt pool solidification	Microstructure evolution	Microstructure study

As it can be seen from table 2, different simulation methods are listed with the suitable application areas within the L-PBF process. The various physical phenomena occurring in the L-PBF process along with the specific areas of application for the simulation methods have been listed.

4 SIMULATION SOFTWARE

Simulation software have been developed by various organizations to understand the laser beam and material interaction at micro and mesoscale. Among many different software, Flow 3D from Flow Science has been developed to understand the powder spreading and melt pool formation by utilizing a combination of DEM and CFD methodology. Flow3D uses DEM to simulate the spreading of the powder particles on the powder bed and CFD to simulate the melt pool formation [50]. ANSYS Additive provides a multiscale simulation approach for the user to understand the L-PBF process from microscale to macroscale. ANSYS utilizes multiple modules like CFD, FEA and FEM to simulate different aspects of the L-PBF like powder spreading, laser beam and material interaction, residual stress and distortion [51]. Digimat from Hexagon is a software which is under development that focuses on material development from an atomistic scale to microscale based on integrated computational materials engineering [52]. Additive Lab has an unnamed software in development which uses thermo-mechanical CFD models to study the melt pool at mesoscale [53]. Amphyon is a mesoscale software that predicts the thermal history of the L-PBF [54]. Figure 5 summarizes the different software in use for mesoscale and microscale simulation of L-PBF.

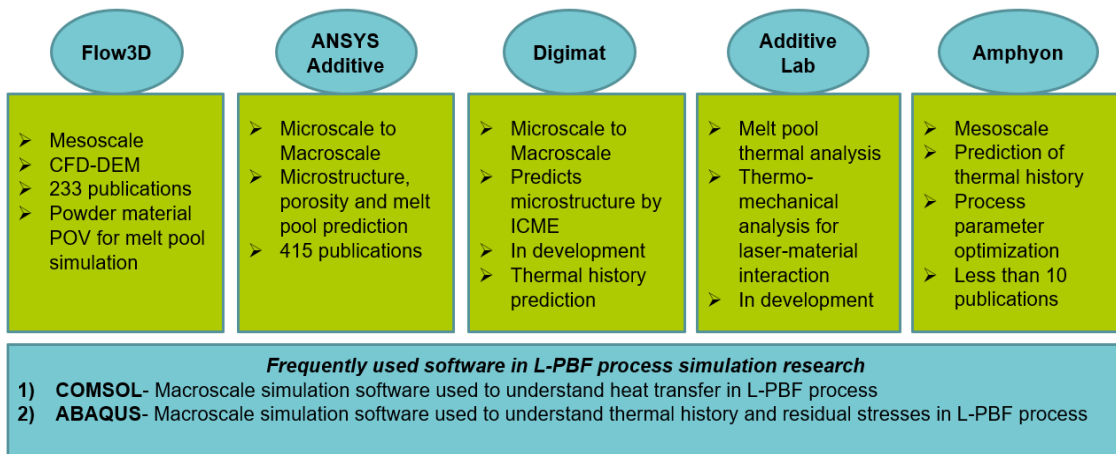


Figure 5. Different simulation software used in L-PBF

As figure 5 shows, various softwares are presented with respect to length scale, physical phenomena and their impact on research in melt pool study of L-PBF. A comparison of different

upcoming softwares is illustrated along with the description of the frequently used software in the area of laser beam and material interaction for L-PBF.

5 CHALLENGES WITH MICRO AND MESOSCALE SIMULATION

The scope of simulation software in the recent years has expanded to microscale and mesoscale level from macroscale level [55]. Simulation of physical phenomena occurring in L-PBF on microscale and mesoscale allows for a larger control over the L-PBF process. This means that the data obtained from the simulation allows for parameter optimization and process control and improves the process [56]. Simulation data can be used for testing the L-PBF process instead of conducting an experiment with a given set of parameters. The entire L-PBF process is simulated which allows for removal of design of experiments which is used for improving the efficiency of the process.

Simulation of the L-PBF process, irrespective of the scale at which it is performed, requires validation before it can be used directly for research [57]. Validation of a simulation is a method where the data gathered from simulation is compared with the results from the experiment. This is done via mechanical testing and in-situ process signal detection. Multiple iterations of simulation need to be carried out before the results agree with the experimental data, as seen in the approaches of different researchers [58], [59]. This is a limitation when using simulation for the optimization of L-PBF process, which suggests that simulation is not at a level where it can completely remove the experimental aspect of research and development of L-PBF process. The need for experimental validation of simulation and vice versa in order to optimize the L-PBF process indicates a gap that exists between simulation and real time iterations of the process. The gap suggests that until the simulation software is at an optimum level, the application of simulation for L-PBF will always need to include experimental validation of the simulation results.

6 CONCLUSION

The aim of this study was to identify the importance of micro and mesoscale simulation in L-PBF process. Simulation in L-PBF is usually performed at macroscale or part scale level. The purpose of conducting this study is to understand the possibility to improve the understanding of the laser beam and material interaction at microscale and mesoscale level by the use of simulation.

Literature review was conducted in the field of simulation in L-PBF for the laser beam and material interaction. From this review, it was found out research regarding the simulation of laser beam and material interaction at micro and mesoscale level is lacking when compared to the simulation at a part scale level. A background study was conducted on the existing research on simulation at micro and mesoscale level and the use of simulation at this scale was justified. An insight was provided into the simulation methods at micro and meso scale level with suitable methods suggested for different physical phenomena occurring in the L-PBF process. This was then followed by an analysis of existing software and their impact on research in this field was studied.

The main conclusion from this study is that there is a clear gap between the research on simulation at part scale in L-PBF and simulation at micro and mesoscale level. The findings of this study indicate the procedure that needs to be followed to conduct simulation at micro

and mesoscale level. An FEM-DEM or an FVM-DEM combination of simulation provides qualitative results for studying the physical phenomena occurring during the L-PBF process. The thermal history of the process combined with the PF model is the method followed by different researchers to simulate microstructure at meso scale level. It was also concluded that among the existing software, COMSOL and ABAQUS have been used frequently followed by newly developed software like Flow3D and Amphyon. The main used to compare different software here are the number of existing publications where the software have been used. A brief description of challenges while using simulation has been presented where experimental validation of the simulation has been identified as a key challenge.

As further studies based on this study, it is concluded that there is need for developing a methodology for using simulation at micro and mesoscale level to understand the laser beam and material interaction in a qualitative manner and improve the L-PBF process by using the data from this.

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