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Qian Liu

A Thesis in fulfilment of the requirements for the degree of Master of Philosophy

School of Mechanical and Manufacturing Engineering

Faculty of Engineering

November 2020
In this study, a machine-learning approach based on Gaussian process regression was developed to identify the optimized processing window for laser powder bed fusion (LPBF). Using this method, we found a new and much larger optimized LPBF processing window than was known before for manufacturing fully dense AlSi10Mg samples (i.e., relative density $\geq 99\%$). The newly determined optimized processing parameters (e.g., laser power and scan speed) made it possible to achieve previously unattainable combinations of high strength and ductility. The results showed that although the AlSi10Mg specimens exhibited similar Al-Si eutectic microstructures (e.g., cell structures in fine and coarse grains), they displayed large differences in their mechanical properties including hardness (118 - 137 HV 10), ultimate tensile strength (297 - 389 MPa), elongation to failure (6.3 - 10.3\%), and fracture toughness (9.9 - 12.7 kJ/m$^2$). The underlying reason was attributed to the subtle microstructural differences that were further revealed using two newly defined morphology indices (i.e., dimensional-scale index $I_d$ and shape index $I_s$) based on several key microstructural features obtained from scanning electron microscopy images. It was found that in addition to grain structure, the sub-grain cell size and cell boundary morphology of the LPBF fabricated AlSi10Mg also strongly affected the mechanical properties of the material. The method established in this study can be readily applied to the LPBF process optimization and mechanical properties manipulation of other widely used metals and alloys or newly designed materials.
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Abstract

In this study, a machine-learning approach based on Gaussian process regression was developed to identify the optimized processing window for laser powder bed fusion (LPBF). Using this method, we found a new and much larger optimized LPBF processing window than was known before for manufacturing fully dense AlSi10Mg samples (i.e., relative density ≥ 99%). The newly determined optimized processing parameters (e.g., laser power and scan speed) made it possible to achieve previously unattainable combinations of high strength and ductility. The results showed that although the AlSi10Mg specimens exhibited similar Al-Si eutectic microstructures (e.g., cell structures in fine and coarse grains), they displayed large difference in their mechanical properties including hardness (118 - 137 HV 10), ultimate tensile strength (297 - 389 MPa), elongation to failure (6.3 - 10.3%), and fracture toughness (9.9 - 12.7 kJ/m²). The underlying reason was attributed to the subtle microstructural differences that were further revealed using two newly defined morphology indices (i.e., dimensional-scale index \( I_d \) and shape index \( I_s \)) based on several key microstructural features obtained from scanning electron microscopy images. It was found that in addition to grain structure, the sub-grain cell size and cell boundary morphology of the LPBF fabricated AlSi10Mg also strongly affected the mechanical properties of the material. The method established in this study can be readily applied to the LPBF process optimization and mechanical properties manipulation of other widely used metals and alloys or newly designed materials.
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1. Introduction

Laser powder bed fusion (LPBF), as one of the most popular metal-based additive manufacturing (AM) technology [1], is a rapid prototyping technique using laser beam to selectively melt and fuse metallic powders layer by layer guided by computer-aided design (CAD) data. Compared to conventional manufacturing methods such as casting and forging, LPBF is considered to have a great potential in industry applications due to its unique and significant advantages including geometrical design freedom, short lead times and performance enhancement [2, 3]. To date, it has been successfully applied in components manufacturing of various industrial fields such as aerospace, medical and automotive industries [4-6].

Due to the complex physical and chemical processes involved in LPBF and the different microstructure-property relationships for each metal or alloy [7, 8], identification of the optimized LPBF processing parameters usually relies on a costly and time-consuming trail-and-error process consisting of a large number of experiments. Some rational methods for LPBF process optimization have been reported, including empirical laser energy density estimation [9], melt pool structure analyses [10], and high fidelity computational modelling [11, 12]. Using optimized LPBF processing parameters, it is possible to achieve high quality fabricated parts (i.e., fully dense and crack-free) for a number of metallic materials, including Al and Ti light alloys [13-16], Ni-based superalloys [17], steels [18], metal-based matrix composites (MMCs) [19], metallic glasses (MGs) [20], shape memory alloys (SMAs) [21], and high entropy alloys (HEAs) [22, 23]. However, the optimization process remains highly problematic and challenging, particularly when a new metal or alloy is to be designed or adopted for LPBF production. More importantly, current process optimization approaches give only a very limited
number of specific sets of processing parameters for the fabrication of fully dense specimens, rather than exhaustively searching the entire high-density optimized processing window which may reveal a wider range of desired properties for a given metal or alloy. This lack of a robust method of optimizing the processing parameters is currently a major barrier to the further development of the LPBF technology and the associated design of materials for specific properties.

Recently, machine learning (ML) has emerged as a new approach for LPBF processing parameter optimization. For example, Wang et al. [24] proposed neural network (NN) machine learning as a useful tool to predict the density of parts. However, while NN is a powerful technique, it generally needs a relatively large training data set to achieve an accurate prediction, which is costly and time-consuming for the LPBF process. Fang et al. [25] reported that support vector machine (SVM) models can provide an effective method for predicting alloy aging behavior, but SVM shows certain limitations when using smaller data sets [26]. In contrast to NN and SVM, Kamath & Fan [27] have proposed Gaussian process regression (GPR) as a competitive model for solving optimization problems with small data sets, which can also provide the uncertainty of the prediction. Moreover, Tapia et al. used GPR for predicting single track melt pool depth [28] and part density using a small range of input data (i.e., 10 W laser power range and 125 mm/s scan speed range) [29], thereby indicating its great potential as a cost-effective solution to the LPBF processing parameter optimization problem.

In addition to density, LPBF process optimization also needs to consider key quasi-static and dynamic mechanical properties, such as tensile properties, fracture toughness, and fatigue resistance [30-33]. It is widely observed that the same metal or alloy fabricated to
comparably high density (> 99%) using different processing parameters can exhibit significant differences in mechanical properties. For instance, the ultimate tensile strength may vary from 168 to 455 MPa in LPBF fabricated AlSi10Mg parts with > 99% relative density [34]. The underlying reason for this phenomenon is attributable to differences in their microstructures but the details are still poorly understood and further research on the microstructure-property relationships is needed.

Therefore, this thesis aims to provide a new paradigm of LPBF process optimization and manipulation of the microstructure for desired mechanical properties in an AlSi10Mg alloy. This new approach combined the machine-learning algorithm, specifically Gaussian process regression (GPR), to identify the optimized LPBF processing window for this alloy. Two of the most critical LPBF parameters, laser power \((P)\) and scan speed \((v)\), were selected as GPR inputs to build a relationship between the processing parameters and the relative density, which then enabled quick identification of the optimized processing window for achieving high density in AlSi10Mg. Then, the microstructure characterization of AlSi10Mg was conducted with the help of image processing method and statistical analysis. Specifically, using a principle component analysis (PCA), ten microstructure morphology features obtained from scanning electron microscopy images were reduced into two new microstructure description indices, denoted as the dimensional-scale index \((I_d)\) and the shape index \((I_s)\). The relationships between the key microstructural features and mechanical properties were finally discussed and determined within the optimized LPBF processing window.
2. Literature Review

2.1. Background

Additive manufacturing (AM), also known as Rapid Prototyping [35], is defined and classified into seven categories by the American Society of Testing and Materials (ASTM), among which laser powder bed fusion (LPBF) is wildly used due to its capability of fully melting the metal powder and the great performance of end-use parts made by it [5, 36]. Compared to conventional manufacturing methods, LPBF is considered to have great potential due to its unique and significant advantages including geometrical design freedom, short lead times and performance enhancement [2, 3], based on an incremental layer-by-layer manufacturing process as shown in Figure 1. For the past decade, LPBF has been experiencing a rapid development has been applied in components manufacturing of various industrial fields such as aerospace, medical and automotive industries [4-6].

![Figure 1. Layer-by-layer LPBF process. (i) High-power laser melts selective areas of the powder bed. (ii) Process repeats for successive layers. (iii) Loose powder removed and finished part revealed. [36]](image)

To date, there have been quite a few types of metals designed and applied in LPBF. The most commonly used materials include iron-based alloys, titanium alloys, aluminum
alloys, nickel-based alloys and so on. The applications of different materials usually depend on their unique properties and the material cost. For instance, iron-based alloy can be used for fabricating heat exchangers with complex geometry or in a mini size [37]. Moreover, due to the light weight (small relative density) and high strength, titanium and its alloy are usually in the medical and aerospace field [38]. In this thesis, we mainly focus on the aluminum alloy, specifically AlSi10Mg due to its high strength to density ratio, high corrosion resistance and castability. This alloy is commonly used for various applications, such as engine parts and cover plate, especially with complicated geometry structure. Moreover, there have been a few works related to optimal parameters in SLM for AlSi10Mg, which can be used for comparison with the optimization results from this thesis.

2.2. LPBF processing parameters

With the growing importance of laser powder bed fusion (LPBF) technique, there is an increasing interest from both academia and industries regarding how to fabricate metallic materials with high density or quality. The process optimization is always the major hurdle in the path of LPBF applications due to more than 60 processing parameters needed to be optimized for fabrication [39]. The most studied parameters are laser power ($P$), scan speed ($v$), hatching space ($h$) and layer thickness ($t$) [40-43], which are illustrated in Figure 2. Optimization of four parameters mentioned before is commonly considered as the most important mission in the application of specific components with better quality and properties or the first requirement of new 3D printing material development to get a proper process window for consulting. Improper parameter combination leads to various of issues and eventually result in poor quality of components. For instance, a detrimental balling phenomenon takes place in case of insufficient energy, which is usually related to
fast scanning speed, insufficient laser power and thicker layer [44]. On the other hand, too much energy density is detrimental as well due to the following evaporation issue and keyhole-mode melting phenomenon [45], resulting in recoil pressure on the melt pool [46] and increasing voids respectively. Additionally, a large hatching distance between two scanning line may lead to regular porosity in components due to insufficient overlap of two adjacent melt pool [36].

Figure 2. LPBF process illustrations for different process parameters. [36]

In the early stage, single tracking scanning experiments could always give some preliminary hints of suitable processing parameters by analyzing melt pool cross-section (e.g., height and width) [10, 41, 47]. For instance, to generate the scanning overlap between adjacent layers/tracks for fully melting the powder into solid, the height of the melt pool can indicate appropriate layer thickness used for part fabrication while the hatching space can be estimated by the width of melt pool. Furthermore, some studies focused on optimizing processing parameters targeting on fabricated part density directly for various of alloys such as AlSi10Mg [42, 48], iron-based alloy [49], titanium alloy [50].
and so on. However, most of previous optimization approaches for LPBF rely on a costly
trail-and-error process and a large number of experiments.

To simplify the optimization process, people proposed laser energy density (ED) as a
useful indicator to evaluate the processing parameters at the same time [9, 17], which is
defined as:

\[
E = \frac{P}{v \cdot h \cdot t}
\]  

(1)

where \( P \) is laser power (W), \( v \) is scan speed (mm/s), \( h \) is hatch distance (mm), and \( t \) is
layer thickness (mm) [51]. According to the expression, the energy density will reflect
the laser energy transferred to powder per volume per time, so that one can adjust the
processing parameters based on a suitable ED value. However, it has been reported by
Prashanth et al. [52] that the ED indicator is not reliable or suitable at all time. For instance,
the metal powder cannot be fully melted with too low laser powder no matter how to
adjust other processing parameters. Moreover, a too fast scan speed will introduce balling
phenomenon even if a suitable ED is used [53].

It is worth noting that even though LPBF technologies provide ideal mechanical
properties and high accuracy of complex parts [54], it is still limited to small parts due to
a low manufacturing speed (up to 105 cm\(^3\)/h with four lasers) [55]. Therefore, a suitable
set of processing parameters with high scanning speed is highly desired in the industry,
which makes process optimization as one of the most important tasks in this LPBF
application.
2.3. Machine learning approaches applied in LPBF process optimization

Current process optimization approaches give only a very limited number of specific sets of processing parameters for the fabrication of fully dense specimens, rather than exhaustively searching the entire high-density optimized processing window which may reveal a wider range of desired properties for a given metal or alloy. This lack of a robust method of optimizing the processing parameters is currently a major barrier to the further development of the LPBF technology and the associated design of materials for specific properties. Recently, machine learning (ML) has emerged as a new approach for LPBF processing parameter optimization. For example, Regression tree algorithm was proposed by Kamath [56] and the accuracy of the model is reasonable if there were enough sample points (seen in Figure 3), and it can be further improved by improving sampling of design space using Poisson-disk sampling [57] and Mitchell’s best-candidate sampling [58]. However, the accuracy will drop dramatically when it comes to a small data set training situation.

Random stratified; 10 trees

![Graph showing the accuracy of the regression tree model in predicting the depth.][56]

Figure 3. The accuracy of the regression tree model in predicting the depth. [56]
Moreover, Wang et al. [24] proposed neural network (NN) machine learning as a useful tool to predict the density of parts. ANN method combined with genetic algorithm (GA) is proved to be applicable in other AM technology field for finding relation between input parameters and concerned output value and searching the global optimum parameters [59, 60]. The configuration of the ANN model in [60] is shown in Figure 4. However, while NN is a powerful technique, it generally needs a relatively large training data set to achieve an accurate prediction, which is costly and time-consuming for the LPBF process.

![Figure 4. The configuration of neural network model. [60]](image)

In addition, Fang et al. [25] reported that support vector machine (SVM) models can provide an effective method for predicting alloy aging behavior, but SVM shows certain limitations when using smaller data sets [26].

In contrast to previously mentioned models, Kamath & Fan [27] have proposed Gaussian process regression (GPR) as a competitive model for solving optimization problems with small data sets, which can also provide the uncertainty of the prediction. As shown in Figure 5, Gaussian process regression model can maintain a relatively higher predicting accuracy with only limited training data, which is more applicable in LPBF process optimization due to less experimental cost for less required sample quantity. Moreover,
Tapia et al. used GPR for predicting single track melt pool depth [28] and part density using a small range of input data (i.e., 10 W laser power range and 125 mm/s scan speed range) [29], thereby indicating its great potential as a cost-effective solution to the LPBF processing parameter optimization problem.

Figure 5. Predicted versus actual values for the length, depth, and width for the Eagar–Tsai-462 data set and the depth using the Eagar–Tsai-100 data set for the different surrogate models using a leave-one-out approach. From top to bottom: MARS multivariate adaptive regression splines, SVR support vector regression, and GP Gaussian processes. [27]
2.4. Simulation approaches applied in LPBF process optimization

With the continuous improvement of computer technology, the applicability of simulation methods has improved and has been used in some research. Kamath [40, 56] introduced a simple Eagar-Tsai model [61] to simulate the depth of melt pool, so that a rough suitable scope of parameters can be obtained. However, the error of E-T model result even reached around 50% compared to real experimental data [56]. The author also proposed a more complex physical simulate model, Verhaeghe model [62], for improving the accuracy of simulation results. Even though the accuracy significantly improved, the model with more physics taken into consideration is more computationally expensive. Moreover, there are more simulation methods introduced in LPBF technique such as finite element analysis (FEA) [63], Lagrangian–Eulerian (ALE) techniques [64] and finite volume method (FVM) [12]. Although all these works focused on single track simulation, they were still time-consuming. Therefore, the main limitation of simulation approach is high computationally cost and difficulties of modelling entire SLM process for a part.
2.5. Mechanical properties of LPBF alloys

![Graphs showing mechanical properties](image)

Figure 6. (a) Room temperature tensile stress-strain curves of the as-built SLM samples that solution heat-treated at different temperatures; (b) corresponding mechanical data; (c) tensile test stress-strain curves of the solution + artificial aging specimens; (d) the Vickers hardness of the as-built and heat-treated SLM specimens. [65]

In addition to the density of fabricated parts, some key quasi-static and dynamic mechanical properties (e.g., tensile, fatigue, etc.) of the LPBF fabricated metallic specimens were also heavily researched [30, 31]. Recently, other key mechanical behaviors of LPBF fabricated metallic specimens including crack propagation and fracture toughness are also explored in this field [32, 33]. For instance, Li et al. [65] optimized the post-heat treatment targeting on tensile properties of fabricated specimens as shown in Figure 6. For instance, after the post-heat treatments, the strength of the LPBF parts generally will decrease while the elongation tends to be better. Moreover, it is
widely observed that the same metal or alloy fabricated to comparably high density (> 99%) using different processing parameters can exhibit significant differences in mechanical properties. For instance, the ultimate tensile strength may vary from 168 to 455 MPa in LPBF fabricated AlSi10Mg parts with > 99% relative density [34]. The underlying reason for this phenomenon is attributable to differences in their microstructures but the details are still poorly understood and further research on the microstructure-property relationships is needed. Therefore, density should not be the only indicator for the quality of LPBF fabricated parts and more mechanical properties should be taken into consideration.

2.6. Microstructure characterization

Due to the high cooling rate during the LPBF process, the LPBF fabricated alloys generally have the different and unique microstructures compared to traditional fabrication approach such as casting such as cellular-dendritic structure in Al-Si alloys [66], different δ-phase distribution in Inconel 718 [67] and acicular α´martensitic microstructure in CP-Ti [68]. These unique microstructure features caused by high cooling rate solidification are the most convincing proof of higher mechanical performance compared to casting counterpart [40, 69]. Taking AlSi10Mg as an example (seen in Figure 7 and Figure 8), special scanning track patterns can be observed from a large-scale view while the fine cellular structure and different grain patterns can be found after zooming in.
Figure 7. Microstructure of an AlSi10Mg SLM part in top view by SEM. Top view SEM micrographs of a sample produced with long bidirectional scanning tracks. The sample was etched with Keller’s. The location of pictures A-C are indicated on the top left picture. In picture C, the melt pool zone with fine (“MP fine”) and more coarse (“MP coarse”) structure are indicated as well as the heat affected zone (“HAZ”). [70]
Figure 8. EBSD orientation maps in two perpendicular views for an AlSi10Mg SLM part. EBSD maps of the front view (left) and top view (middle) of sample B. The scanning and building direction is indicated by the black arrows on the pictures and some of the melt pool borders are pointed out by the dashed lines. The specimen coordination system and the crystal orientation–color relation map referenced to the direction perpendicular to TD and RD are shown at the right. [70]

In general, scanning electron microscope (SEM) and Electron backscatter diffraction (EBSD) are the most common techniques to characterize the sub-grain microstructure and grain microstructure respectively, as shown in Figure 7 and Figure 8. However, to quantify the microstructure characterization, current approaches mainly focus on length-scale measurements such as average cell size or cell spacing [71, 72] (Figure 9), or a statistical index generated from a two-point spatial statistics algorithm which can
represent the microstructure morphology [73, 74]. There is still a lot of information being lost or ignored during quantification process.

![Diagram of LPBF process](image)

Figure 9. Method to compute the cell size with the melt pool depth from Rosenthal's and Matyja's equation. [71]

### 2.7. Conclusion

It can be seen that the LPBF AlSi10Mg has a great potential for both material research and industry applications due to its superior properties and geometry design freedom of additive manufacturing technique. The process-structure-property linkage of this alloy has been studied with different approaches, but the quantitative relationship has not been fully understood yet. A new machine-learning assisted LPBF process optimization approach and the manipulation of the microstructure for desired mechanical properties in an AlSi10Mg alloy will be proposed in the following sections in order to address the hurdle of AlSi10Mg manufacturing and applications.
3. Methodology

3.1. Powder material and LPBF process

Gas atomized AlSi10Mg powder with a diameter between 20 and 63 µm supplied by LPW Technology Ltd was used in this study; the chemical composition of the powder is shown in Table 1. All the AlSi10Mg specimens in this thesis including cubes, tensile bars and compact tension (CT) specimens were fabricated on an SLM Solutions 125HL machine (seen in Figure 10), equipped with a 400W continuous wavelength (CW) fiber laser with a wavelength of 1060 nm. The process was carried out under a high purity Ar gas atmosphere (oxygen content $\leq 0.02$ at%) to avoid oxidation. The build plate was pre-heated to 200°C for all the LPBF experiments to relieve residual stress in fabricated specimens and further reduce distortion [75]. Two of the most important LPBF processing parameters, laser power and scan speed, were chosen as variables in this study while the other processing parameters were fixed (see Table 2). The bidirectional scanning strategy was applied with a 90° scan angle increment between layers. Laser energy density, $E$ (J/mm$^3$), was calculated for each parameter combination.

Table 1. Chemical composition of the AlSi10Mg alloy (wt.%).

<table>
<thead>
<tr>
<th></th>
<th>Al</th>
<th>Si</th>
<th>Mg</th>
<th>Fe</th>
<th>O</th>
<th>Zn</th>
<th>Mn</th>
<th>Cu</th>
<th>Ni</th>
<th>Pb</th>
<th>Sn</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bal</td>
<td>9.9</td>
<td>0.38</td>
<td>0.13</td>
<td>0.08</td>
<td>&lt;0.1</td>
<td>&lt;0.01</td>
<td>&lt;0.05</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.2</td>
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</table>

Table 2. LPBF processing parameters in this study

<table>
<thead>
<tr>
<th>Processing parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laser Power (W)</td>
<td>100, 130, 160, 190, 220, 250, 280, 310, 340, 370, 400</td>
</tr>
<tr>
<td>Scan speed (mm/s)</td>
<td>500, 750, 1000, 1250, 1500, 1750, 2000, 2250, 2500</td>
</tr>
<tr>
<td>Hatching Space (µm)</td>
<td>100</td>
</tr>
<tr>
<td>Layer thickness (µm)</td>
<td>30</td>
</tr>
</tbody>
</table>
3.2. Gaussian process regression

Gaussian processes regression (GPR) was chosen to build a relationship between the relative density of fabricated parts and the LPBF processing parameters, i.e., laser power and scan speed in this study. GPR (also known as Kriging in statistics) is an interpolation method based on a Gaussian process where the collection of random variables has a joint Gaussian distribution with a continuous domain [76]. The density ($\rho$) of a specimen fabricated using a laser power $P$ and scan speed $v$ can be described by its mean function and covariance function (or kernel) [76]:

$$\rho(P,v) = GP(m(P,v), k(P,v,P',v'))$$  \hspace{1cm} (2)

where $\rho(P,v)$ denotes the relative density from the training data points $(P,v)$ and predicting points $(P',v')$. The hyperparameters in $m(P,v)$ and $k(P,v,P',v')$ can be trained using the input data so that the density value corresponding to a new processing
parameter set \((P', v')\) can be predicted as a Gaussian distribution with mean value and variation. For mathematical convenience purpose, data preprocessing was applied in two steps: (i) the processing parameters (i.e., laser power and scan speed) were normalized to be non-dimensional. This step enabled the use of the popular squared exponential (SE) kernel for the covariance function without considering the different units of the inputs; (ii) Then, the relative density values of the training data set were normalized to zero mean. The training dataset consists of 82 combinations of laser power and scan speed are listed in Table 2. Details of the learning process and results are presented in Section 0 and readers referred to [76] for more mathematical details about the GPR process.

### 3.3. Chemical composition analysis

The chemical composition of LPBF fabricated AlSi10Mg specimens were quantitatively measured using inductively coupled plasma atomic emission spectroscopy (ICP-AES, Agilent 5110 Dual View, seen in Figure 11). This spectroscopy detects elements by producing excited atoms and ions from plasma that emits electromagnetic radiation at wavelengths characteristic of a particular element.

Figure 11. Agilent 5110 Dual View system
3.4. Microstructure characterization

The sub-grain microstructures of the AlSi10Mg specimens were characterized using a Nova NanoSEM 450 field-emission scanning electron microscope (FE-SEM). For sample preparation, all specimens were progressively ground to a P4000 SiC paper finish and then polished using 3 µm and 1 µm diamond solutions. Weck’s reagent, which is composed of 4 g KMnO₄, 1 g NaOH and 100 ml distilled water, was used to reveal the eutectic and cellular microstructure in AlSi10Mg. SEM images of all the specimens used in the image processing work (Section 3.5) were taken using the same settings of 12,000× magnification, a working distance of 5.6 mm, an acceleration voltage of 5 kV, and a spot size of 3.0 to ensure high consistency in image region and quality. Moreover, after mechanical tests, the fractured surfaces of both tensile test and fracture toughness specimens were examined using the same FE-SEM set-up.

The grain microstructure of the AlSi10Mg was further characterized by electron back-scattered diffraction (EBSD) using a Carl Zeiss AURIGA CrossBeam Workstation with a step size of 0.35 µm. All specimens were prepared the same as SEM samples but without the etching step.

3.5. Image processing and microstructure quantification

In order to uncover and characterize the subtle features in the microstructure of LPBF fabricated AlSi10Mg, an image processing approach was designed, as illustrated in Figure 12.
Figure 12. Illustration of the image processing steps. The original SEM image is first converted into a binary image. Dots inside the cells are removed (red circle area) and small breakpoints of the network structure are fixed (red rectangle area). Each closed black cell was treated as analytical unit region hereafter.

A grey-colored SEM image (Figure 12a) is first converted to a binary image (Figure 12b), which represents different phases separately (i.e., Si-rich phase in white and \( \alpha \)-Al phase in black). A denoising operation is then applied to remove white noise (e.g., the noise in the red circled area in Figure 12b) while maintaining the dominant structural integrity of the Al cells. Subsequently, discontinuities of the Si precipitate network are considered as lost details during binary processing (defined as < 3 pixels, see an example in the red rectangle area in Figure 12c) and fixed by using binary morphological operation. Each closed black cell was regarded as the isolated region representing an analytical unit for the following morphology feature analysis. Based on previous studies [77-79], ten morphological features were carefully selected to represent the detailed microstructural characteristics of each cell, which are listed in Table 3.

Table 3. Morphological features extracted for microstructure description

<table>
<thead>
<tr>
<th>Variable</th>
<th>Feature</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X_i )</td>
<td>Area</td>
<td>The number of pixels in the region</td>
</tr>
<tr>
<td></td>
<td>Feature</td>
<td>Description</td>
</tr>
<tr>
<td>---</td>
<td>---------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>$X_2$</td>
<td>Perimeter</td>
<td>Distance around the boundary of the region (in pixels)</td>
</tr>
<tr>
<td>$X_3$</td>
<td>Major Axis Length</td>
<td>Length of the major axis of the ellipse region (in pixels)</td>
</tr>
<tr>
<td>$X_4$</td>
<td>Minor Axis Length</td>
<td>Length of the minor axis of the ellipse region (in pixels)</td>
</tr>
<tr>
<td>$X_5$</td>
<td>Roundness $^a$</td>
<td>Roundness feature of a profile defined as $4\pi (\text{Area})/(\text{perimeter})^2$</td>
</tr>
<tr>
<td>$X_6$</td>
<td>Convexity $^b$</td>
<td>Proportion of pixels in the convex hull that are not in the region</td>
</tr>
<tr>
<td>$X_7$</td>
<td>Aspect Ratio</td>
<td>The ratio of the major axis to the minor axis</td>
</tr>
<tr>
<td>$X_8$</td>
<td>Eccentricity $^c$</td>
<td>The ratio of the distance between the foci of the ellipse and its major axis length</td>
</tr>
<tr>
<td>$X_9$</td>
<td>Rectangularity $^d$</td>
<td>The area ratio of the white region to its bounding box</td>
</tr>
<tr>
<td>$X_{10}$</td>
<td>Tortuosity $^e$</td>
<td>The ratio of major axis to perimeter</td>
</tr>
</tbody>
</table>

a. Roundness demonstrates the similarity of a region to a perfect circle. A value closer to 1 indicates a higher similarity.

b. Convexity reflects the integrity of the cell. It is a non-negative number and a greater value indicates a more convex hull structure. A larger convexity often demonstrates the incompleteness of the border.

c. Eccentricity is a value between 0 and 1. The closer it is to 1, the flatter the ellipse-like shape.

d. Rectangularity is the property of being shaped like a rectangle. Equal to 1 if the shape is rectangular, otherwise less than 1. This indicator can also be used to describe the gross similarity of a region to an ellipse.

e. Tortuosity is the ratio of the maximum linear length between any two points on the contour to the contour length. A smaller tortuosity indicates a shape with a more tortuous boundary.

For quantifying the morphological information carried by each SEM images, every individual black cell was regarded as a unit, where ten-features would be extracted. As
listed in Table 3, some of the features are, to some extent, sharing partially overlapped capabilities in morphological description. For instance, although not linearly associated, a larger Area would often indicate a greater Major axis length for a region in SEM images. Such overlapping would inevitably result in a redundant description, which is not preferred, regarding the enormous data to be analyzed. To reduce data redundancy and thus enable a more efficient microstructure description, the ten feature descriptors shown in Table 3 were reduced using a principal component analysis (PCA), after which the information was transformed into an updated, lower dimensional space. Specifically, new weighted morphology indices $Y_1, ..., Y_{10}$ with different weight scores were computed with a polynomial expression as shown in Eq. (3):

$$Y_i = b_{i1} \cdot X_1 + b_{i2} \cdot X_2 + b_{i3} \cdot X_3 + \ldots + b_{i10} \cdot X_{10}, \ i \in [1, 10]$$  \hspace{1cm} (3)

The coefficients $b_i$ reflect the contribution of each microstructural feature to the related morphology index. As the morphology index with a larger score contains more useful information [80], new weighted morphology indices with high scores will be chosen to represent the statistical characteristic information of microstructure in this study.

### 3.6. Density measurement

For relative density measurement, AlSi10Mg cubes (5×5×5 mm3) were built using the range of processing parameters listed in Table 2. Density was measured using the Archimedes method with an A&D Weighing HR-250A balance. The solid specimens were weighed in air ($w_a$) first and then again in the distilled water ($w_b$). The density of the solid specimen ($\rho$) can be calculated as follows:

$$\rho = \frac{w_a}{w_a - w_b} (\rho_0 - \rho_a)$$  \hspace{1cm} (4)
where $\rho_0$ and $\rho_a$ are the density of distilled water and the air at measuring temperature, respectively. In order to reduce experimental error, three samples were measured for each parameter set and a theoretical density of 2.67 g/cm$^3$ was used.

### 3.7. Mechanical properties tests

The cubic specimens were used for hardness test. The hardness of specimens was measured using a Buehler 1100 Series Macro Vickers hardness tester according to ASTM E92 standard [81]. The Vickers scale and test force were fixed at HV 10 and 10 kgf, respectively. Dog-bone shaped specimens with a cross section of 2×4 mm and a gauge length of 18 mm were fabricated for tensile testing. Compact tension (CT) specimens for fracture toughness were cut from LPBF fabricated plates (32×33×10 mm) using electrical discharge machining (EDM). Both tensile and CT specimens were oriented such that the loading direction would be perpendicular to the build direction (BD), a configuration known to yield the best combination of mechanical properties (i.e., tensile strength and fracture toughness) according to previous studies [82, 83]. Tensile tests were conducted on an Instron 3369 Machine according to the ASTM E8 standard [23], at a displacement rate of 1 mm/s at room temperature. A 12.5 mm gauge extensometer was used for tensile strain measurement, and a calibrated 50 kN load cell was used for force measurement. Following the ASTM E1820 standard [84], elastic-plastic fracture toughness tests were performed on an Instron 8872 machine with a clip gauge for displacement measurement and a 25 kN load cell for force measurement. All CT specimens were pre-cracked by applying a stress intensity range ($\Delta K$) of 7 MPa-m$^{1/2}$ with a frequency of 50 Hz and load ratio (R) of 0.1. The single specimen method was used whereby cracks were extended from pre-cracks followed by a series of unloading/reloading cycles to define the J-R curve, which is a measure of fracture toughness that incorporates plastic deformation as
compared to the predominantly linear-elastic $K_{IC}$ testing method. The hardness, tensile and fracture toughness values were averaged from at least three samples.

Figure 13. Tensile bar (left) and CT specimen (right) dimensions (mm) and the building direction (above); the set-ups of tensile test (left) and fracture toughness test (right) with extensometer and clip gauge respectively (below)
4. Results

This chapter presents the results of process optimization targeting density of LPBF AlSi10Mg, microstructure characterization and outstanding mechanical performance compared to previous studies. The GPR optimizing model and corresponding result are shown in Section 4.1 and 4.2. Microstructure characterization with new morphology description indices is presented in Section 4.3. And further discussions about process-structure-property relationship are presented in Section 4.4, 4.5 and 4.6.

4.1. GPR model for the relative density contour map

Figure 14. Symbols indicate the training data for the average and standard deviation of the relative density at discrete parameters of laser power and scan speed. Processing parameters resulted in printing failures (e.g., keyhole and lack-of-fusion) were excluded and some examples of failed prints are shown in the insets.

The relative density of the AlSi10Mg specimens fabricated using different processing parameters (Table 2) are plotted in Figure 14. These relative density values were used as the training dataset to create a predictive density surrogate surface (Figure 15) by fitting the GPR method as described in Section 3.2. It should be mentioned that data points
corresponding to part build failures (inset images in Figure 14) during LPBF are excluded from the training dataset. In this study, the observed printing failures were mainly attributed to severe defects of keyhole, balling or bead-up phenomena [45, 85, 86], mostly caused by inferior LPBF processing parameters, e.g., low laser power and high scan speed (insufficient energy input) or the opposite (excessive energy input). These inadequate parameters correspond to the two corners indicated in Figure 14. One of the unique features of GPR is the ability to provide the uncertainty of the prediction; one standard deviation indicating the error band of predictions is presented in Figure 16. As shown in the figure, prediction error in relative density is less than 0.3% over a large range of possible processing parameters, indicating the high accuracy of the GPR model. In addition, extrapolation errors are clearly visible in Figure 16 in the two corners outside the training data range. Since the predicted relative density in these two corner regions is less than 95%, the relatively large error is of little practical significance. For validation of the GPR model, a validating data set was created, as detailed in Section 4.2 below.
Figure 15. Response surface of the GPR predicted relative density mean value.

Figure 16. Relative density prediction uncertainty represented by one standard deviation from predictive mean value. The relatively high extrapolation error can be found at two corners where no training data were available.
Establishing an optimized material processing window to achieve high relative density is of fundamental importance to successful LPBF fabrication of metals and alloys. One previous approach to identify such window was proposed by Johnson et al. [87], where they used a single scan track geometry thermal model to develop a printability map for Ni with 5 wt.% Nb and CoCrFeMnNi high entropy alloy. In this study, we made further progress from optimizing single scan track behavior to optimizing bulk specimen density, and from a descriptive problem-based processing map (e.g., keyhole, balling and lack-of-fusion areas) to a more accurate predictive relative density contour map. Assisted by the GPR model, a much larger optimized LPBF processing window can be determined with limited experimental data as input (Figure 15), which provides a wide range of previously unexplored processing parameters for fabricating fully dense AlSi10Mg (i.e., relative density > 99%).

4.2. Optimized LPBF processing window for AlSi10Mg

Based on the relative density contour map obtained in Figure 15, the range of LPBF processing parameters that can be used to fabricate AlSi10Mg specimens with a relative density > 99% was defined as the optimized LPBF processing window hereafter (as denoted by the orange area in Figure 17a). For comparison, the optimized processing parameters for AlSi10Mg reported in the literature [10, 31, 41, 69, 88-97] are also shown in gray areas in Figure 17a. Interestingly, the optimized processing window predicted in this study is significantly larger than the ranges reported in previous studies (within the same laser power range ≤ 400 W). This implies that there exists a much wider range of optimized parameters for fabricating fully dense AlSi10Mg specimens. It is expected that this newly established optimized processing window would potentially uncover more opportunities for fabricating AlSi10Mg parts with both high density and desired
microstructures and mechanical properties, which will be shown and discussed in the following sections.

Figure 17. a Relative density contour map as a function of laser power and scan speed. Energy density lines (dotted line) represent the same laser energy density based on Eq. (1). The orange area denotes the newly identified processing window to achieve > 99% relative density using the machine-learning method in this study, which is larger than those identified in previous studies (gray shaded areas). A set of five new parameter sets, denoted by the yellow stars (as detailed in Table 4), were chosen from the newly established optimized processing window as the validation data set and used for subsequent microstructure and mechanical properties study; b Measured relative density values for the five validating data points compared to the predicted values from the GPR model. Error bars indicate one standard deviation. The relative densities of all five specimens are between 99.2% and 99.4%, as indicated by the red band.
Table 4. Validation data set of five processing conditions (within the optimized processing window) for following microstructure and mechanical properties studies

<table>
<thead>
<tr>
<th>Name</th>
<th>subgroups</th>
<th>Laser Power (W)</th>
<th>Scan speed (mm/s)</th>
<th>Energy Density (J/mm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E38</td>
<td>1</td>
<td>264</td>
<td>2320</td>
<td>38</td>
</tr>
<tr>
<td>E51/P300*</td>
<td>1,2</td>
<td>300</td>
<td>1960</td>
<td>51</td>
</tr>
<tr>
<td>E70</td>
<td>1</td>
<td>355</td>
<td>1690</td>
<td>70</td>
</tr>
<tr>
<td>P200</td>
<td>2</td>
<td>200</td>
<td>1307</td>
<td>51</td>
</tr>
<tr>
<td>P355</td>
<td>2</td>
<td>355</td>
<td>2320</td>
<td>51</td>
</tr>
</tbody>
</table>

* E51 and P300 represent the same LPBF parameters. We use two names here with the aim to simplify our discussion below.

To validate the GPR model, five different processing conditions within the optimized processing window were selected (details in Table 4) as the validation data set which is independent of the training set in Figure 14. Cubic samples (8×8×8 mm³) of each of the five processing conditions were fabricated for density measurement and microstructure analysis. As shown in Figure 17b, for specimens fabricated using the validation data set, the measured relative densities agreed very well with the values predicted by the GPR model with an error less than 0.3%. All the measured values locate within the error bar, indicating the high accuracy of the GPR predictions. It is also worth pointing out that the five processing conditions correspond to three different energy densities $E$, as shown in Figure 17a. They are treated as two subgroups for the following detailed studies on microstructure and mechanical properties. The first group (E38, E51 and E70) compares the influence of different laser energy densities on the AlSi10Mg specimens while the second group (P200, P300 and P355) focuses on the effect of different laser power and scan speed combinations when using the same laser energy density 51 J/mm³.
The shape of the established optimized processing window (i.e., the orange area in Figure 17a) can be rationalized by considering the following mechanisms for porosity formation during LPBF. Combinations of high speed and low power (in the top left corner in Figure 17a) lead to insufficient energy to fully melt powders. By contrast, the keyhole phenomenon dominates at low speed and high power (bottom right corner in Figure 17a), which is consistent with Ref. [87]. Additionally, it is worth noting that the optimized processing window in the relative density contour map becomes wider towards the higher laser power and speed region (top right corner in Figure 17a) when compared with lower power and speed region (bottom left corner in Figure 17a). This can probably be attributed to the higher laser power induced expulsion mechanism during LPBF which is known to expel spatters and suppress related defects, further enlarging the suitable range of laser scan speed at high laser power for fabricating fully dense parts using LPBF [11].

4.3. Microstructure of the LPBF fabricated AlSi10Mg

The sub-grain fibrous microstructures of the AlSi10Mg specimens fabricated using the optimized parameters in Table 4 are shown in Figure 18a. All specimens exhibit a typical eutectic and cellular Al-Si microstructure observed from a cross-section perpendicular to the build direction. Importantly, although the specimens were fabricated using very different processing parameters in terms of laser power and scan speed (see Table 4), the specimens display very similar microstructures with no major differences. Representative melt pool tracks from the LPBF process are also shown in Figure 18b and c for a typical P355 specimen. Figure 18d shows the detailed microstructural features near the melt pool boundary where three different regions are observed which can be defined as fine, coarse and heat affected zone (HAZ) based on their different cell size and morphology. Most cells in the fine region have a size range within 0.5 - 1 µm, while the cell size in the coarse
region is larger than 2 µm. Discontinuous Si precipitates can be found in HAZ. The melt pool core area exhibited a sub-grain cellular microstructure which is typical for LPBF fabricated Al-Si alloys [70] where the α-Al matrix is surrounded by a network of Si precipitates, as shown in Figure 18e. The grain microstructures of the five specimens shown in the EBSD inverse pole figure (IPF) maps in Figure 19 exhibit a small difference in grain size with no other difference in their microstructures. Corresponding average grain sizes (d) for the specimens are listed in Table 5.

Figure 18. a SEM images showing the eutectic and cellular Al-Si microstructures in the AlSi10Mg fabricated using the five processing conditions in Table 4. b Optical microscope image and c SEM image of melt pool structures. d Melt pool boundary microstructure with fine, coarse regions and heat affected zone (HAZ). e Typical LPBF fabricated AlSi10Mg microstructure in the melt pool core area with dark α-Al matrix decorated with bright Si precipitates. For figures b-d, only a P355 specimen is shown as a representative of all the five AlSi10Mg specimens.
Figure 19. EBSD map of the AlSi10Mg specimens fabricated using the five processing conditions in Table 4. The color code representing the crystal orientation is included.
Table 5. Grain size, morphology indices $I_d$ and $I_s$ and mechanical properties of the AlSi10Mg specimens fabricated using the LPBF parameters listed in Table 4

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Average Grain Size (µm)</th>
<th>$I_d$</th>
<th>$I_s$</th>
<th>Yield Strength (MPa)</th>
<th>UTS (MPa)</th>
<th>Elongation (%)</th>
<th>Hardness (HV$_{10}$)</th>
<th>$J_{IC}$ Value (kJ/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E38</td>
<td>3.95 ± 2.85</td>
<td>-0.62</td>
<td>0.64</td>
<td>228.7 ± 3.3</td>
<td>388.8 ± 4.9</td>
<td>6.3 ± 0.6</td>
<td>137.3 ± 2.0</td>
<td>9.9 ± 0.6</td>
</tr>
<tr>
<td>E51/P300</td>
<td>4.24 ± 3.37</td>
<td>0.17</td>
<td>-0.19</td>
<td>183.7 ± 0.9</td>
<td>359.1 ± 2.9</td>
<td>10.3 ± 0.3</td>
<td>124.1 ± 1.0</td>
<td>11.4 ± 0.5</td>
</tr>
<tr>
<td>E70</td>
<td>5.81 ± 5.02</td>
<td>0.33</td>
<td>-0.23</td>
<td>144.3 ± 1.8</td>
<td>297.5 ± 1.6</td>
<td>9.5 ± 0.9</td>
<td>118.4 ± 1.3</td>
<td>12.7 ± 0.6</td>
</tr>
<tr>
<td>P200</td>
<td>4.77 ± 3.77</td>
<td>-0.16</td>
<td>0.04</td>
<td>208.3 ± 3.9</td>
<td>386.9 ± 4.4</td>
<td>8.6 ± 0.6</td>
<td>130.6 ± 2.1</td>
<td>11.4 ± 0.7</td>
</tr>
<tr>
<td>P355</td>
<td>4.23 ± 3.19</td>
<td>0.28</td>
<td>-0.25</td>
<td>190.3 ± 4.0</td>
<td>364.1 ± 6.3</td>
<td>8.3 ± 1.2</td>
<td>127.1 ± 1.9</td>
<td>11.8 ± 0.5</td>
</tr>
</tbody>
</table>
As seen in Figure 18, all specimens exhibit similar morphology features with typical eutectic and cellular microstructure consisting of a network of $\alpha$-Al with Si precipitates. To characterize this microstructure, current approaches mainly focus on length-scale measurements such as average cell size or cell spacing [71, 72], or a statistical index generated from a two-point spatial statistics algorithm which can represent the microstructure morphology [73, 74]. In this study, we took ten morphology features into consideration to develop two new morphology indices ($I_d$ and $I_s$) for characterizing AlSi10Mg cellular microstructure.

To uncover the key differences in the observed microstructures of the AlSi10Mg specimens, a total of 96 SEM images of the melt pool microstructures were taken for each specimen listed in Table 4. A total of 200,000 $\alpha$-Al cells were randomly selected from the 96 SEM images per specimen to remove any bias. The ten features from Table 3 were then calculated for each cell to build a microstructure analysis database. After a principal component analysis (PCA, Section 3.3), the main microstructure morphology information was reduced to a lower feature dimension, and resultant coefficients are listed in Table 6. Based on the feature contribution coefficients, two new microstructure morphology indices were introduced. The first morphology index captures the effect of structure size (i.e., area, major axis length and perimeter) and shape fullness (i.e., roundness and convexity) and is thus defined as the dimensional-scale index ($I_d$). A larger value of $I_d$ implies universally bigger cells in the microstructure that on average contain more convex hull structure, because a small cell perimeter does not have the line length needed to form a convex hull shape. The second morphology index is related to shape (e.g., aspect ratio and eccentricity) and boundary details (e.g., tortuosity), and is thus termed as shape index ($I_s$). A larger $I_s$ mainly indicates a slimmer cell structure with a rougher boundary. It is
worth noting that $I_d$ (weighted 59% from the PCA process) is substantially more influential than $I_s$ (weighted 26%).

<table>
<thead>
<tr>
<th>Features</th>
<th>Coefficients</th>
<th>Corresponding value in $I_d$</th>
<th>Corresponding value in $I_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area</td>
<td>$b_1$</td>
<td>0.3653</td>
<td>-0.1998</td>
</tr>
<tr>
<td>Perimeter</td>
<td>$b_6$</td>
<td>0.3930</td>
<td>-0.1570</td>
</tr>
<tr>
<td>Major Axis Length</td>
<td>$b_2$</td>
<td>0.3955</td>
<td>-0.0116</td>
</tr>
<tr>
<td>Minor Axis Length</td>
<td>$b_3$</td>
<td>0.2942</td>
<td>-0.3907</td>
</tr>
<tr>
<td>Roundness</td>
<td>$b_4$</td>
<td>0.3790</td>
<td>0.0070</td>
</tr>
<tr>
<td>Convexity</td>
<td>$b_5$</td>
<td>0.3637</td>
<td>0.0366</td>
</tr>
<tr>
<td>Aspect Ratio</td>
<td>$b_7$</td>
<td>0.2429</td>
<td>0.4658</td>
</tr>
<tr>
<td>Eccentricity</td>
<td>$b_8$</td>
<td>0.2293</td>
<td>0.4436</td>
</tr>
<tr>
<td>Rectangularity</td>
<td>$b_9$</td>
<td>-0.2829</td>
<td>-0.1695</td>
</tr>
<tr>
<td>Tortuosity</td>
<td>$b_{10}$</td>
<td>-0.0402</td>
<td>0.5820</td>
</tr>
</tbody>
</table>

Based on $I_d$ and $I_s$, we constructed a bivariate histogram descriptor shown as the spot intensity for each specimen (Figure 20a). A clear difference in the spot intensity is observed among the abovementioned five specimens (Table 4), indicating different microstructural morphology features were formed in the AlSi10Mg specimens fabricated using the five processing conditions. Due to the equal amount of data used to construct each histogram (i.e., 200,000 $\alpha$-Al cells), a higher intensity spot represents a more concentrated distribution based on the two morphology indices $I_d$ and $I_s$, denoting that the specimen tends to have a more uniform microstructure. Moreover, the mean values were calculated for both indices ($I_d$ and $I_s$) and the center points of each histogram corresponding to each specimen are marked in Figure 20b. In general, E38 has the higher
intensity spot with a smaller $I_d$, indicating that it has a more uniform microstructure across the whole specimen and its cell structure tends to be smaller, rounder and have less concave portion.

Figure 20. **a** Visualization of the microstructure characterization of the LPBF fabricated AlSi10Mg based on the dimensional-scale and shape indices. A higher intensity spot implies a more uniform microstructure across the whole specimen. The color bar representing the absolute frequency of the cell unit in bivariate histogram is included. **b** Center of histograms and schematic interpretation for mean values of the morphology indices $I_d$ and $I_s$. 
4.4. Relationship between solidification process and new morphology indices

Based on the indices $I_d$ and $I_s$, we propose a modified relationship to understand the influence of LPBF processing parameters on the microstructure from a cooling rate perspective. For example, regarding the dimensional-scale index ($I_d$) in Figure 20, the size of $\alpha$-Al cells is previously considered inversely proportional to the cooling rate ($P^k$) [98]. When considering the solid-liquid interface where solute-rich boundary forms during solidification process, the cooling rate $P^k$ as a function of laser power and scan speed (Eq.(5)) can be derived from Rosenthal’s equation (Eq. (4)):

$$\frac{2\pi(T - T_0)kR}{Q} = \exp\left[\frac{-v(R - x)}{2\alpha}\right]$$

(5)

by calculating the time derivative of temperature between the liquidous, $T_l$, and the solidus, $T_s$, temperatures to arrive at:

$$P^k = 2\pi k(T_s - T_0)(T_l - T_s)\frac{v}{Q}$$

(6)

where $T_0$ is the build plate temperature, parameter $R$ is the radial distance, $x$ is the distance on scanning direction from the origin, $k$ is the thermal conductivity of AlSi10Mg, $\alpha$ is the workpiece thermal diffusivity, $v$ is the laser scan speed and $Q$ is the heat transferred from laser into powder. However, the above relationship cannot explain the difference in the second comparative sub-group in Table 4 (P200, P300 and P355), in which specimens have the same ratio of $v/P$. Based on [99], the deposited heat in the powder $Q$ should be revised to equal the laser power $P$ times the laser absorptivity $\beta$ as presented in Eq. (6):

$$\frac{P^k}{Q} = \frac{v}{\beta P} \propto \frac{v^{1.5}}{P^2}$$

(7)
Following this, the rank order of the cooling rates for the five AlSi10Mg specimens in this study is $I_{E38} > I_{P200} > I_{E51/P300} > I_{P355} > I_{E70}$, which is in good agreement with the inverse relationship to $I_d$. As shown in Eq. (7), the size of the cell structures (including area, perimeter and major axis length) is proportional to the cooling rate and can be tailored using different laser power and scan speed.

It is also worth noting that there is a correlation between $I_d$ and $I_s$. As shown in Figure 20, a larger dimensional-scale index tends to evolve into a circle-like cell but with a more complex boundary. Because the expansion of the solid-liquid (S/L) interface during the solidification process in all directions would become more isotropic with increasing time, the aspect ratio of cells tends to decrease as cooling rate decreases. Meanwhile, a longer unstable S/L interface (i.e., a larger cell perimeter in $I_d$) has more opportunity to deform from a planar interface to a rugged interface, which affects the complexity of cell boundaries. Additionally, with more cooling time, the convex hull structure (shown in Figure 20) is more likely to occur due to incomplete small cells merging process during solidification [98].

4.5. Mechanical properties of the LPBF fabricated AlSi10Mg

The hardness and tensile tests for the two sub-groups of the AlSi10Mg specimens (Table 4) are shown in Figure 21, and the detailed values for each mechanical property are summarized in Table 5. Moreover, it can be seen that with increasing laser energy density from 38 to 70 J/mm³ (E38, E51 and E70), yield strength increases from 144 to 229 MPa, ultimate tensile strength (UTS) from 297 to 389 MPa, and hardness from 116 to 134 HV
In general, the E38 parameters gave the highest mechanical strength and hardness. When using the same energy density of 51 J/mm$^3$ (P200, P300 and P355), the difference in measured hardness and strength was relatively small (Table 5). This indicates that for the LPBF fabricated fully dense AlSi10Mg specimens the mechanical properties were mainly controlled by the overall laser energy density while varying the laser power ($P$) and scan speed ($v$) under identical energy density conditions have limited influence.

In addition, three $J$-$R$ curves were obtained for each sub-group from the fracture toughness tests. For visualizing convenience, they are shown in Figure 22 as an average curve with standard deviation (shaded areas), while average and standard deviation of the separately calculated $J_{IC}$ values for each test are shown in Table 5. Generally, the fracture toughness was found to be inversely proportional to both yield strength and hardness.
4.6. Improved mechanical properties and fracture mechanisms

Figure 22. J-R curves of AlSi10Mg specimens fabricated using the five optimized LPBF processing parameters conditions in Table 4.

Figure 23. Summary of the UTS and elongation of LPBF fabricated AlSi10Mg in previous literature, compared to the AlSi10Mg specimens in this study. The arrow
schematically illustrates what could previously achieved by post heat treatments, while the circled stars show our results that achieve previously unattainable, yet highly desirable, properties without post heat treatment.

As seen in Figure 17, the larger processing window has the potential to enable the design of LPBF processes that can achieve both high density and previously unattainable mechanical properties (i.e., a combination of higher UTS and elongation). The UTS and elongation from the literature [10, 31, 33, 65, 69, 88-90, 94, 97, 100-114] are summarized in Figure 23, including material that has been heat treated after processing. Most of the as-built specimens have high tensile strength but low ductility. The arrow schematically illustrates the evolution of mechanical properties by post heat treatment, resulting in improved ductility while sacrificing tensile strength [65]. In this study, by exploring an optimized LPBF processing window, AlSi10Mg parts with previously unattainable, yet highly desirable, combinations of high strength and elongation without post heat treatment (see in Figure 23) can be achieved.

![Figure 24](image.png)

**Figure 24.** Si phase proportion (solid histogram) and chemical composition analysis (stripe histogram) in the AlSi10Mg specimens fabricated using the five selected optimized LPBF processing conditions in Table 4.
In order to understand the underlying mechanisms for the observed differences in the mechanical properties among the five AlSi10Mg specimens in Table 5, a few critical microstructural features such as grain size, sub-grain microstructure (i.e., cell structure) and the fraction of secondary phase (i.e., Si precipitation) were considered [115]. These microstructural features are generally related to the known strengthening mechanisms in metallic materials [81]. As shown in Figure 24, both the fraction of Si network calculated by image analysis and the silicon proportion in element composition measured using the ICP-AES method were similar among the five specimens, which indicates that the fraction of Si is probably not a major influential factor to cause the observed differences in mechanical properties. With regards to grain boundary strengthening mechanisms (or Hall-Petch strengthening effect $\Delta \sigma_{\text{Hall-Petch}} = k d^{-1/2}$), the low $R$-squared ($R^2$) value of 0.52 from yield strength - $d^{-1/2}$ single variable regression (Figure 25) indicates the grain boundary strengthening alone cannot fully explain the large differences in mechanical properties. Similarly, the new microstructure morphology indices are insufficient to fully explain the variability on their own (e.g., the dimensional-scale index in Figure 25). However, a multiple variable regression on the combination of grain size and the two new morphology indices ($I_d$ and $I_s$) does a much better job to explain the strength variability as evidence by the much higher coefficient of determination of $R^2 > 0.92$. This indicates that the strength is controlled by both the grain size and the sub-grain microstructure (i.e., cell structure). The role of grain size on strength in the LPBF fabricated AlSi10Mg is a well-studied field; therefore, the following discussion will mainly focus on the sub-grain microstructure, which is also regarded as one of the main reasons for the enhanced strength in LPBF fabricated AlSi10Mg compared with its cast counterparts.
Figure 25. Single variable regression on dimensional-scale indices (left and middle) and $d^{-1/2}$ (right) respectively based on five studied specimens.

Figure 26. Side view of tensile test specimens (a) and fracture toughness test specimens (b) showing the cracks with respect to the melt pool structure; fractographs indicate typical ductile fracture with dimples on both E38 and E70.
Consistent with the idea proposed by Delahaye et al. that the melt pool boundary is a relatively weak portion compared to the fine cell structure in the melt pool core area [71], some crack path deviations triggered by melt pool boundaries were observed during the fracture toughness experiments in this study (Figure 26). However, observations of the tensile and fracture toughness test specimens revealed a combination of crack propagation paths along the melt pool boundaries and throughout the melt pool cores. When a crack is confined to the melt pool core regions, the cell structure provides the main resistance to crack growth. The Si network, regarded as precipitation hardening mechanism, also has a significant influence on the fracture mechanism. Based on fractography, ductile fracture with dimple rupture feature can be observed across the entire fracture surface for both E38 and E70. The general size of the dimples around 0.5-1 µm (shown for E38 and E70 in Figure 27) is consistent with the cell size in the core melt pool area, which also agrees with the findings reported by Delahaye et al. [71]. However, a very low ductility ~1.8% due to failure occurring in the artificially enlarged heat affected zone of the melt pool boundary was reported in Ref. [71]. In contrast, in the present study the ductility was much higher (6.3 - 10.3%) and failure most often occurred within the melt pools. These differences are attributed to the different build orientations between these studies, whereby in Ref. [71] the loading axis was parallel to the build direction and the melt pool boundaries ran along the cross section of each specimen, providing easy sites for failure to initiate in the coarser cells near the melt pool boundary.
Moreover, according to [116], the dislocations usually pile up at cell boundaries under tensile loading, resulting in local hardening. Specifically, for finer cells, the accumulative dislocations and stress concentrations would have a higher tendency to be evenly dispersed throughout the specimen as a result of more interfaces between phases per unit volume. On the other hand, for coarser cells, the convex hull structure which breaks the integrity of cell structures would also introduce more local stress concentrations. The critical local stress for micro-void nucleation in continuum plasticity model is
\[
\sigma_c = \sigma_m + \bar{\sigma}_{\text{max}}, \quad \text{where } \sigma_m \text{ and } \bar{\sigma}_{\text{max}} \text{ are the macroscopic mean-normal stress and maximum local tensile stress on the interface, respectively [117]. Thus, when E70 has a larger } I_d \text{ (indicating larger cells and more convex hull structures), more stress concentration causes the increase of } \bar{\sigma}_{\text{max}}, \text{ making it easier to reach } \sigma_c \text{ for void nucleation and eventually leading to fracture.}
\]
5. Conclusions

In this thesis, a machine-learning approach based on the GPR model has been proposed to identify the optimized LPBF processing window for fabricating fully dense AlSi10Mg and the relationship between the LPBF processing parameters, microstructures and mechanical properties has been investigated. The following conclusions can be drawn:

(1) The GPR surrogate model is an effective approach to building a model for the effects of laser power and scan speed on relative density of LPBF fabricated AlSi10Mg. This model makes it possible to identify a larger optimized LPBF processing window than previously explored one for fabricating AlSi10Mg to high relative density ($\geq 99\%$). Rather than providing one specific optimized parameter set, an optimized processing window with a predictable high relative density contour map can be identified using the model. The approach provides huge potential for designing LPBF fabricated AlSi10Mg with microstructures that result in desired mechanical properties such as high strength and ductility which was unattainable before.

(2) Two new morphology indices, i.e., the dimensional-scale index ($I_d$) and the shape index ($I_s$), have been defined by applying a principle component analysis to ten microstructural morphology features, which can better characterize the sub-grain microstructure of the LPBF fabricated AlSi10Mg. Moreover, a relationship between $I_d$ and processing parameters (i.e., laser power and scan speed) has been derived to enable tailoring the microstructure by controlling processing parameters.

(3) The mechanical properties of AlSi10Mg specimens fabricated using optimized LPBF parameters have been found to depend primarily on energy density, while the different combinations of laser power and scan speed will introduce minor variations. Differences in their mechanical properties were mainly attributed to the different
grain size and sub-grain microstructure morphology. The dimple size on the fracture surfaces is related to the sub-grain cellular structure size in the melt pool core areas, which were found to provide paths of low crack propagation resistance in addition to the weak melt pool boundaries.
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