Understanding Structure-Processing Relationships in Metal Additive Manufacturing via Featurization of Microstructural Images

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Abstract

Understanding and predicting accurate property-structure-processing relationships for additively manufactured components is important for both forward and inverse design of robust, reliable parts and assemblies. While direct mapping of process parameters to properties is sometimes plausible, it is often rendered difficult due to poor microstructural control. Exploring the direct relationship between processing conditions and microstructural features can thus provide significant physical insights and aid the overall design process. Here, we develop an automated high-throughput framework to simulate an uncertainty-aware additive manufacturing (AM) process, characterize microstructural images, and extract meaningful features/descriptors. A kinetic Monte Carlo (KMC) model of the AM process is used as a digital twin to simulate microstructural evolution for a diverse set of experimentally relevant processing conditions. We perform a detailed parametric study to map the relationship between microstructural features and experimental conditions. Our results indicate that a many-to-one mapping can exist between processing conditions and typical descriptors. Multiple descriptors are thus necessary to unambiguously represent microstructural images. Our work provides crucial quantitative and qualitative information that would aid in the selection of features for microstructural images. Featurized microstructures could then be utilized to build data-driven models for predictive control of microstructures and thereby properties of additively manufactured components.

1. Introduction

Additive manufacturing (AM) has proven to be a superior candidate, when compared to traditional manufacturing processes such as subtractive and near-net-shape processes, for producing intricate and sophisticated parts with complex geometries [1, 2]. Additive manufacturing (AM) is a transformative technique that allows layer-by-layer creation of components with complex geometries which are prohibitively difficult to achieve with traditional manufacturing techniques. For example, additively manufactured Ti-6Al-4V components that are lighter and stronger are being incorporated into existing and new turbine engine designs for aerospace applications. The mechanical properties of such components are highly sensitive to the underlying microstructure, which depends strongly on the manufacturing process conditions.

Unlike conventional manufacturing, AM is a complex history dependent process; a workpiece is built up using a material feedstock, such as powder or wire, and a targeted energy deposition source, such as an electron beam or laser. The supplied energy melts the feedstock to create a small pool of liquid metal, which solidifies as the source moves away. Some combination of the feedstock, energy source, and workpiece are rastered to move the melt pool, building the workpiece in three dimensions. Final microstructure and hence the mechanical property of AM samples is a strong function of processing parameters. AM process parameters are mostly tuned by trial-and-error which is time consuming, costly, highly subjective, and machine- and material-specific. Process control of microstructure remains elusive. Currently, our understanding of microstructure development in AM alloys such as Ti-6Al-4V derives from simple heat treatment studies, with thermal paths similar to those used in conventional manufacturing.
Complex thermal history (melting, solidification, phase transformation during cooling and post-deposition annealing) leads to poor control and uncertainties, i.e., significant deviation from desired microstructures. Knowing the structure-property-processing relationship is highly desirable, but it has remained a challenge to map important and relevant features in microstructures to the processing conditions.

Additive manufacturing for producing metal parts can be classified into two categories, Powder Bed Fusion (PBF) [3] and Direct Energy Deposition (DED) [4]. In the PBF process, a laser spot traverses across the powder bed, that results in melting and subsequent solidification of the powder bed. Using this technique, several layers of metal can be deposited. In the DED technique, building multiple layers on a substrate depends on the nature of the feedstock delivery through the nozzle and laser power [4]. Feedstock can be powder or a wire. DED typically uses a single or a co-axial nozzle to deliver feedstock to an energetic source (laser), and a shielding gas to resist oxide formation. The moving laser spot creates a thermal gradient between the substrate and deposited layers during the solidification process, which creates a rapid cooling rate resulting in microstructural heterogeneity. A combination of elongated and equiaxed grains can be found due to varying thermal gradients along a single laser pass or scan pattern. Control over the overall manufacturing process, both PBF and DED, is typically achieved by manipulating the shape of laser spot, power input, and trajectory of the laser. Furthermore, uni-directional, bi-directional, and crosshatch between adjacent laser passes allow finer control over the obtained grain morphology. Mechanical and thermal properties of the final product [5, 6] is strongly correlated with the underlying microstructure, which in turn depends on the additive manufacturing process parameters - laser velocity, dimensions of laser spot, etc. Therefore, understanding relationship between the process parameters of AM and the resulting microstructure is crucial for designing components with desired properties.

Researchers have experimentally explored the effect of process parameters on different morphologies of grains [7–11]. These prototypical experimental explorations not only incur significant monetary costs but are also prohibitively time consuming. With the advancement of computational capabilities and numerical methods, in-silico experimentation can result in higher throughputs and rapid prototyping of different components associated with AM. Metal additive manufacturing processes have similarities with the welding process; thus, most of the state-of-the-art models for grain growth during the additive manufacturing process have been motivated from the existing numerical models for welding [12]. Cellular Automata coupled with Finite Element [13] and Lattice Boltzmann method-based temperature models [14] are some of the few popular methods in this domain. Few empirical models [15] also have been used for the estimation of microstructural features that collect information from the thermal history generated from the thermal simulation performed. Phase-field models are another popular choice for simulating additive manufacturing microstructures [16–18] but possess certain limitations regarding the coarsening of grains in the heat affected zone (HAZ) region and incur high computational cost [19].

In recent past, the Kinetic Monte Carlo (KMC)-based Potts model [20] for grain evolution has been developed to circumvent some of the aforementioned bottlenecks and accurately simulate additively manufactured microstructures. The KMC Potts model is based on simulation technique that approximates polycrystalline microstructure with the help of curvature-driven grain growth. Multiple
passes of the heat source along a three-dimensional or a two-dimensional domain can be simulated using this methodology. This model has been used by Rodgers et al. [21] to simulate welding and additive manufacturing problems. Recently, the KMC-based microstructure simulation framework for additive manufacturing [22] has been improved and a conduction solver based on finite difference method has been incorporated to create an integrated tool for the representation of nucleation and solidification of grains [23]. The KMC Potts model was also used by Li et al. [24, 25] to simulate grain morphology in the DED process. They studied the effect of different scanning patterns, i.e., uni-directional and bi-directional scanning patterns, and transverse speeds of the laser on the resulting microstructure.

One of the most important aspects of any AM process is the characterization of microstructures. Several algorithms exist for characterizing these microstructures [27, 28], including modern data-driven techniques [29–31]. Although, the KMC Potts model has been proven to be very efficient for creating microstructures for AM processes [20–26], detailed characterization and analysis of microstructural images obtained from these simulations is lacking. Furthermore, due to the inherent stochasticity in these models, one-to-one comparison of microstructural images is infeasible. Robust featurization, accounting for stochasticity, of these microstructural images are necessary for obtaining reliable insights from simulated AM processes.

In this work, we address these gaps in knowledge and aim to understand the relationship between the underlying microstructure and the processing conditions via detailed parametric study combined with featurization of microstructural images. We first choose four input processing parameters (velocity, hatch spacing, melt-pool width, and tail length) that have utmost experimental significance. Then we systematically vary these parameters and perform KMC simulations to obtain microstructural images. Finally, we develop quantitative features/descriptors to differentiate between the obtained microstructural images. Our featurization analysis suggests that consideration of more than one feature is absolutely necessary for describing the microstructure accurately. Moreover, the developed features can be used to drive any inverse-design/optimization problem provided appropriate scoring metrics are defined. Our work introduces a robust and automated workflow for the characterization of microstructural images and sets the stage for future inverse design explorations wherein an AM component with tailored mechanical/electrical/thermal properties would be desired. The remainder of the paper is structured as follows. In Section 2, we present the details of the computational technique that we use to simulate additive manufacturing processes (KMC-based Potts model) and describe our automated featurization algorithms followed by results and discussion in Section 4. Finally, in Section 5 we present concluding remarks.

2. Methods

2.1 A Digital twin of the additive manufacturing process: KMC-based Potts model
Experimentally, a few important processing parameters that control an additive manufacturing process include laser beam power, spot size, scan rate, and scan patterns. While it is experimentally challenging to exhaustively explore the effect of all these parameters on the resulting microstructure, the same can be attained in a virtual simulation environment — we thus create a digital twin of the AM process by mimicking the experimental AM process with a KMC based Potts model. We note that these experimental control parameters can be accurately replicated using a combination of computational parameters, such as scan velocity of laser, scanning patterns, and dimensions of melt pool. Figures 1(a) and 1(b) show schematics of our computational model and lists the process parameters considered in this work: hatch spacing (h), scan velocity (v), Melt pool length (l), and Melt pool width (w). Dimensions of the melt pool (l and w) indirectly correlate with experimental process parameters such as laser spot size, scan rate, and the power input. Whereas hatch spacing and scan velocity are direct analogues of experimental process parameters. The heat affected zone (HAZ) depends on the dimension of the melt-pool and the thermal diffusivity of the material. Melt pool depth is another important input parameter of interest in three-dimensional microstructural simulations, but here we restrict ourselves to two-dimensional systems. Three dimensional simulations and corresponding characterization are left for future studies.

As a first step towards a digital twin for AM process, we use a Kinetic Monte Carlo simulation technique based on the Potts model as our computational scheme. The KMC Potts model describes local evolution of grains due to the movement of the molten pool. This model is based on an on-lattice technique where the lattice sites are assumed to be static, and the melt pool moves over the stationary lattice sites. The curvature-driven grain growth is approximated by minimizing the grain boundary energy. The simulation of grain growth using the KMC method is an on-lattice technique [20], where the lattice sites entering inside the molten zone are active and the lattice sites outside the molten zone boundary are inactive and do not take part in the simulation procedure. A detailed description of this methodology can be found in SI.1 and Rodgers et al. [21]. This method has been tremendously successful in replicating experimental AM processes [7, 8]. Hyperparameters that are necessary to define and calibrate the computational model are obtained from Rodgers et al. [20]. After obtaining microstructure images from the KMC simulations, we analyze them using automated featurization algorithms and develop quantitative metrics to differentiate between the different microstructures, as shown in Fig. 1(c). Our overall workflow is described in Fig. 1(d).

### 2.2 Automated featurization algorithms:

With a robust computational model for simulating the AM processes, we can pursue a rapid design and testing of a variety of components. However, without automated and efficient characterization algorithms, the computational methods cannot be utilized to its fullest since it is important to understand the important features in the resulting structures to clearly assess the impact of any given choice of manufacturing processing condition. Moreover, for any inverse design problem involving microstructures, an automated featurization is necessary for high-throughput explorations of the parameter space. In this subsection, we discuss our workflow to allow for automated featurization of microstructure images generated by either KMC simulations or from experiments.
The first step is to analyze the simulated images and extract appropriate descriptors. All simulated images are first analyzed in Python using OpenCV [32], NumPy [33], SciPy [34], Scikit-image [35], and Pandas [36] libraries. Detailed description of our methodology is presented in SI.2. Descriptors from the microstructure images are obtained using custom algorithms and off-the-shelf image processing toolkits, such as the Watershed algorithm [27, 28]. Figure 2(a) delineates our featurization workflow while Fig. 2(b) specifically shows the application of the Watershed segmentation algorithm for separating out individual grains. In Fig. 2(c) and 2(d), we compare our KMC simulation and featurization algorithm with prior studies [8, 21]. More rigorous comparisons and benchmarks are presented in SI.3. Although histograms, shown in Fig. 2(d), are a reasonable visualization method for different descriptors considered in this paper, they can be prone to several artefacts based on the size of bins. To circumvent this issue, we use a kernel density function that approximates the histogram with a continuous function, using kernel density estimation (KDE) [37]. Our kernel density estimation approach is discussed in detail in SI.4. Going forward, we will use these KDE estimates of histograms to compare and analyze different process conditions.

3. Results

The KMC simulation technique along with our automated featurization framework allows us to efficiently explore the parametric space of input parameters, characterize the microstructure images, and extract the relationship between structure and processing conditions. In this study, we focus on variations of scan velocity ($v$), hatch spacing ($h$), Melt pool length ($l$), and Melt pool width ($w$) – parameters which strongly correlate with experimental process conditions. We use a relatively large two-dimensional computational (450x450 sites) domain for our KMC simulations. Based on the dimensions of the molten pool a length scale can be inferred; in our case, a single site is 5 microns [26]. One Monte Carlo Step (MCS) corresponds to an attempt for a spin update with each neighbor of every lattice site. An approximate relationship between MCS and physical time is related by a constant factor [20, 22]. For a given input condition, we perform six independent simulations with varied seed values to capture the effect of stochasticity in KMC simulations.

In Fig. 3, we depict all the different parametric variations considered in this study. A two-dimensional representation of the corresponding simulations is obtained by first featurization of microstructural images and subsequently applying t-SNE (t-distributed stochastic neighbor embedding) [38] dimensionality reduction to these features. More details regarding the t-SNE dimensionality reduction technique and inherent stochasticity in KMC simulations are presented in the supporting information sections SI.5 and SI.6, respectively. Although predominantly meant as a visualization technique, the t-SNE projections highlight certain crucial aspects of our KMC simulations. For each input condition, there are six data points corresponding to different seed values and represented with the same color (see Fig. 3). If the microstructural images across various seed values for a particular input condition are similar, they appear as clusters in the t-SNE plot. Input conditions 1–5 follow this trend, but no such clustering behavior is observed for the remaining input conditions. This observation points to the fact that one instance of a KMC simulation is not reliable and averaging over different seed values are necessary; this
is consistent with any stochastic simulation technique. SI.6 discusses the effect of stochasticity on different descriptors. We next discuss the parametric variations of input conditions in more detail while providing physical insights into the impact of certain key AM process parameters on microstructural features.

### 3.1 Scanning rate and patterns

Velocity of laser spot (scan rate) and hatch spacing (determines the scan pattern) are important process parameters which directly relate to the trajectory of the laser and also possess direct correspondence to experimental setups. Both parameters can significantly influence the microstructural features and therefore warrant detailed investigation.

#### 3.1.1 Velocity of Laser ($v$)

While investigating the effect of velocity variation on microstructural features, we consider velocities of 15, 30, 45, and 60 sites/MCS. Other input parameters are kept constant: $h = 30$, $l = 60$, $w = 45$. More parametric variations are presented in SI.7. Microstructure images for a particular seed are shown in Fig. 4(a). As the velocity increases, the grains become finer and equiaxed in nature. This effect can be observed clearly from the distributions shown in Fig. 4(b).

The orientational distribution, as shown in Fig. 4(b) is bimodal with asymmetric peaks. At larger velocities, the peaks become shallower which illustrates the fact that the grains are less asymmetric and more equiaxed. This observation is further corroborated by the aspect ratio descriptor, which approaches a value of one as velocity increases. While the orientation and aspect ratio descriptors capture the shape variations in a grain, perimeter-area ratio and equivalent diameter describe size variations. As shown in Fig. 4(b), the perimeter-area ratio distribution curves shift towards the right with an increase in velocity. An increase in perimeter-area ratio implies decreasing grain size as perimeter-area ratio scales inversely with grain size. The opposite trend can be observed for the distribution of equivalent diameter - the curves shift leftward with increasing velocity signifying reduction of effective grain size. In all the descriptors shown in Fig. 4(b), prominent quantitative and qualitative differences exist for the considered velocities. Therefore, when developing metrics for distinguishing velocity variations, any one of the four descriptors can be used. However, as discussed later in this Section, we will show that not all descriptors are equally sensitive to all process parameters.

#### 3.1.2 Hatch Spacing ($h$)

The distance between two subsequent laser passes during laser scanning processes (see Fig. 1), i.e., hatch spacing, is an important parameter that strongly influences grain morphologies. Hatch spacings of 20, 40, and 60 sites are used to investigate microstructural variations. Other input parameters have fixed values: $v = 25$, $l = 60$, $w = 45$. More parametric variations are discussed SI.7. The microstructural
morphology variations are shown in Fig. 5(a). When \( h = 20 \), the small spatial separation between the two laser passes limits the lifetime of the fine grains that form just behind the molten region and allows the growth of more columnar grains. As the hatch spacing between the laser passes increases, thin layers of equiaxed grain persist. The distribution-based descriptors shown in Fig. 5(b) corroborates this observation. Orientation, for hatch spacings of 20 and 60 sites, show prominent peaks at angles of ± 70°. The similarity between these two different input conditions can be explained based on the fact that at large enough hatch spacings, highly columnar grains between the equiaxed bands are not stable and break into smaller chunks similar to those obtained with \( h = 20 \). In the mid hatch range, i.e., \( h = 40 \), the distribution flattens as a large number of vertical bands of equiaxed grains exist. Similar conclusions can be made from the aspect ratio and perimeter-area ratio distributions. The curves shift towards the right with a change in hatch spacing from 20 to 40 sites but rescinds left as the hatch spacing increases to 60. The perimeter-area ratio also shows unique bimodal behavior which is indicative of the two types of grains present in these systems. Equivalent diameter captures the overall change in the size of the grains but is not as informative as the perimeter-area ratio distributions.

When investigating the effect of velocity variation on microstructural images, all four descriptors were fairly sensitive to velocity variation. However, in the current scenario for hatch spacing, not all the descriptors are not equally sensitive. Equivalent diameter and aspect ratio cannot distinguish between hatch spacings of 20 and 60 sites. Therefore, a combination of descriptors, especially orientation and perimeter-area ratio, are necessary when developing metrics for distinguishing different microstructural images.

### 3.2 Characteristics of laser spot

Melt pool, the region on the substrate where powder material comes in direct contact with the laser and melts, strongly impacts formation of microstructural morphologies. In our computational model, the shape of the melt pool is characterized by a representative length \( (l) \) and width \( (w) \), as shown in Fig. 1. We investigate the effect of both parameters.

#### 3.2.1 Melt pool width \( (w) \)

Variation of molten pool width of the laser spot significantly impacts the microstructures, as shown in Figs. 6(a) and 6(b). Experimentally, the molten pool width is typically influenced by the laser beam power and scan rate (velocity of the laser). However, in our computational model, we can study the variation of melt pool width independent of other parameters. Three values of \( w \) are considered – 25, 45, and 65 sites; other parameters are fixed at \( v = 25, h = 30, l = 60 \). More parametric variations are presented in SI.7.

Figure 6(b) demonstrates that for higher melt pool widths a vertical laser pass creates a cluster of equiaxed grains. As shown in Fig. 6(c), orientation distribution is smoother at higher pool widths, indicating that the grains are more equiaxed. The aspect ratio descriptor strengthens this finding – the
peak in the aspect ratio distribution approaches one with increasing melt pool width. The bimodal nature
of perimeter-area ratio signifies the existence of grains of two characteristic sizes. When \( w = 25 \), a larger
peak exists at a low perimeter area ratio, which corresponds to grains of larger sizes (columnar grains),
as shown in Fig. 6(b). As \( w \) increases to 45, the major peak occurs at higher ratios indicating that the
fraction of finer grains is higher. At \( w = 65 \), bimodality of this distribution vanishes and points to the
fact that majority of the grains are finer. Variations in equivalent diameter is consistent with perimeter
area ratios, except that the bimodal size distribution of grains is captured less accurately. All descriptors
capture the variations of melt pool width with the perimeter area ratio being the most sensitive amongst
the four.

### 3.2.2 Melt pool length (\( l \))

Other than melt pool width, melt pool length (\( l \)) is another parameter that controls the shape of the laser
spot. \( l \) is varied from 60 sites to 80 sites with increments of 10, and the corresponding effect on the
microstructure is as shown in Fig. 7. More parametric variations for the same are presented in SI.7. In the
considered parametric range, the orientation and aspect ratio distributions are indistinguishable. Thus,
the grain shape does not vary significantly. However, a visible size variation occurs as demonstrated by
the perimeter-area and equivalent diameter distributions: with increasing \( l \), the grain size increases.
Partial bimodality of the perimeter area distribution suggests existence of grains of two sizes at lower
pool lengths.

### 4. Discussion

In this study, we present an automated framework for featurization of microstructural images and aim to
understand the key descriptors and relate them to the input processing conditions. Our workflow and
methodology are agnostic to the specific source of the microstructural images. Although we discuss and
present our analysis using microstructural images generated synthetically using KMC simulations, an
extension to experimentally obtained microstructural images would be straightforward. We perform high-
throughput KMC simulations to probe several important AM processing parameters such as laser beam
power, spot size, scan rate, and scan patterns and analyze the resulting microstructure using an
automated featurization workflow. We show that at least four descriptors/features (aspect ratio, perimter
area ratio, grain orientation, equivalent diameter) are necessary for distinguishing the different
microstructural images generated from parametric variations of the input space. We also demonstrate
that due to the inherent stochasticity of KMC simulations, averaging of features/descriptors over
independent simulations is necessary for obtaining any qualitative or quantitative insights. Error bands
around averaged descriptor distributions capture the stochastic effects of our simulation technique.

As demonstrated by the detailed simulations of grain morphological evolution for various experimental
input or controls, the KMC based digital twins of an additive manufacturing process can model typical
microstructural features observed in AM of metals, such as strong location-dependent distribution of
grain sizes and nonconventional grain shapes and orientations. Due to these unique microstructural
characteristics, empirical relationships (e.g., Hall-Petch relationship) that explain the behavior observed in traditional bulk metals are likely not applicable to AM metals. Machine learning models, with appropriate descriptors, trained on simulated data can be good alternatives for systematically exploring different processing parameters relevant to AM experiments and mapping the relationships between processing, structure/morphology, and materials properties. Despite the use of relatively straightforward descriptors (e.g., grain diameter, orientation, aspect ratio, etc.) that ignore nonconventional shapes, our results have demonstrated that microstructure images can be characterized using distribution curves, which helps us extract structure-processing information from images. Such an approach can be extended to generate descriptors for data-driven models, and it has the flexibility to allow inclusion of more complex microstructural features.

Furthermore, the assessment of variation of input process parameters suggests that a single microstructural feature (i.e.- angular orientation of grains, aspect ratio, perimeter-area ratio, equivalent diameter) is not the sufficient for describing the variations of input parameters; many-to-one mapping exists between inputs and some microstructural features, within the error bars. For e.g., in Fig. 7(b), when molten pool length is varied, the Aspect Ratio and Orientation features are unable to capture any variations. Equivalent diameter captures the variation of melt-pool length well, but it fails when considering variation of hatch spacing in Fig. 5(b) – distributions almost overlap when hatch spacing is 20 and 60 sites. Similarly, the perimeter-area ratio descriptor performs well across all process parameters except for melt pool length. Therefore, multiple features are necessary for unambiguously describing a specific input processing condition.

Another important aspect to note is the inherent stochasticity of KMC simulations; an averaging features/distribution over several independent simulation runs can circumvent this issue. For any optimization or inverse design task, considering mean values of all four descriptors along with the corresponding error bars will be crucial while designing metrics for distinguishing microstructural images. The variations in simulation output results from the use of different random seeds replicates the uncertainties one might observe in repeated experiments or different locations of a sample.

While our high-throughput parametric study and the associated featurization of the microstructure images is in no sense comprehensive, our computational investigations shed light on a few relevant processing parameters which significantly influence microstructural morphologies. From an experimental perspective, the chosen input parameters represent easily tunable or controllable processing conditions. Parametric variation of input parameters and subsequent analysis of the features suggest that typically many-to-one mapping can exist between the input parameters and a specific descriptor. Therefore, multiple descriptors are necessary for unambiguously relating input conditions to microstructural images. Our analysis demonstrates that, while designing metrics for distinguishing microstructural images for any optimization or inverse design task, consideration of at least four descriptors presented in this study (orientation, aspect ratio, perimeter area ratio, equivalent diameter) is necessary. This study lays the groundwork for development of such tailored metrics for uncertainty-aware inverse design problems, which is an interesting avenue for future investigations.
Declarations

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Code and data availability

The KMC code as implemented in SPPARKS Kinetic Monte Carlo Simulator from Sandia National Lab was used in the present study and is publicly available (https://spparks.github.io/). All the code and associated datasets will be made available on reasonable request.

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Authorship contribution statement

DS and AC contributed equally to this project. DS, AC and SKRS conceived the project. DS performed all the KMC calculations with input from AC. DS and AC performed all the feature extraction and data analysis with input from HC and PSD All the authors provided feedback on the workflow and feature extraction. DS, AC and SKRS wrote the manuscript with input from all co-authors. SM, HC, and MC provided feedback on the manuscript. All authors participated in discussing the results and provided comments and suggestions on the various sections of the manuscript. SKRS supervised and directed the overall project.

References


**Figures**

![Figure 1](image)

**Figure 1**

*Schematic representation of the overall computational workflow*(a) Schematic representing the bi-directional scanning pattern of the laser spot and laser trajectory associated process parameters – scan...
velocity and hatch spacing. (b) Schematic representing process parameters that depict the shape of laser spot – melt pool width and melt pool length. (c) Microstructural features (Grain Orientation, Aspect Ratio, Perimeter-Area Ratio and Equivalent Diameter of grains) obtained from the KMC simulations (d) Overall schematic representation of our workflow.

**Figure 2**

*Schematic representation of the automated workflow for featurization of microstructural images and benchmarking with previously published experimental result.* (a) Sequential steps of our automated featurization workflow (b) Input grayscale image and Watershed segmented final image used for measuring the microstructural features of each grain. (c) Comparison of bi-directional additive patterns obtained from the present simulation with experimental results of Nishida et al. [8]. (d) Comparison for distribution of aspect ratio of grains between current study and experimental results of Nishida et al. [8], for the Laser Energy Net Shape (LENS) processing conditions.
Figure 3

Two-dimensional t-SNE representation of all microstructural images considered in this study with the corresponding input conditions. Clustering is observed only for a few processing conditions indicating that stochastic effects of the KMC simulation technique are non-negligible.
Figure 4

Effect of velocity on the microstructure and the corresponding descriptors. (a) Variations in microstructures at different velocities - 15 sites/MCS, 30 sites/MCS, 45 sites/MCS, and 60 sites/MCS. Other input parameters are constant: h=30, l=60, w=45. (b) Descriptors corresponding to the parametric variations. All features are sensitive to velocity variations.

Figure 5
Effect of hatch spacing on the microstructure and the corresponding descriptors. (a) Variations in microstructures at different hatch spacings – 20, 40, and 60 sites. (b) Descriptors corresponding to the parametric variations. Orientation and Perimeter area ratio are most sensitive to variations in hatch spacing.

![Image of microstructures and descriptors](image)

**Figure 6**

Effect of melt pool width on the microstructure and the corresponding descriptors. (a) Variations in microstructures at different melt pool widths – 25, 45, and 65 sites. (b) Microstructural variation in a single pass of the laser over one hatch spacing (c) Descriptors corresponding to the parametric variations. All descriptors are sensitive to variations in melt pool width.
Figure 7

Effect of melt pool length on the microstructure and the corresponding descriptors. (a) Variations in microstructures at different melt pool lengths – 60, 70, and 80 sites. (b) Descriptors corresponding to the parametric variations. Only equivalent diameter is significantly sensitive to variations in melt pool length. Perimeter-area ratio shows mild sensitivity.

Supplementary Files

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