

Strategies for The Characterization and Virtual Testing of SLM 316L Stainless Steel

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ABSTRACT

The selective laser melting (SLM) process allows for the control of unique part form and function characteristics not achievable with conventional manufacturing methods and has thus gained interest in several industries such as the aerospace and biomedical fields. The fabrication processing parameters selected to manufacture a given part influence the created material microstructure and the final mechanical performance of the part. Understanding the process-structure and structure-performance relationships is very important for the design and quality assurance of SLM parts. Image based analysis methods are commonly used to characterize material microstructures, but are very time consuming, traditionally requiring manual segmentation of imaged features. Two Python-based image analysis tools are developed here to automate the instance segmentation of manufacturing defects and subgranular cell features commonly found in SLM 316L stainless steel (SS) for quantitative analysis. A custom trained mask region-based convolution neural network (Mask R-CNN) model is used to segment cell features from scanning electron microscopy (SEM) images with an instance segmentation accuracy nearly identical to that of a human researcher, but about four orders of magnitude faster. The defect segmentation tool uses techniques from the OpenCV Python library to identify and segment defect instances from optical images. A melt pool structure generation tool is also developed to create custom melt-pool geometries based on a few user inputs with the ability to create functionally graded structures for use in a virtual testing framework. This tool allows for the study of complex melt-pool geometries and graded structures commonly seen in SLM parts and is applied to three finite element analyses to investigate the effects of different melt-pool geometries on part stress concentrations.

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GENERAL AUDIENCE ABSTRACT

Recent advancements in additive manufacturing (AM) processes like the selective laser melting (SLM) process are revolutionizing the way many products are manufactured. The geometric form and material microstructure of SLM parts can be controlled by manufacturing settings, referred to as fabrication processing parameters, in ways not previously possible via conventional manufacturing techniques such as machining and casting. The improved geometric control of SLM parts has enabled more complex part geometries as well as significant manufacturing cost savings for some parts. With improved control over the material microstructure, the mechanical performance of SLM parts can be finely tailored and optimized for a particular application. Complex functionally graded materials (FGM) can also easily be created with the SLM process by varying the fabrication processing parameters spatially within the manufactured part to improve mechanical performance for a desired application. The added control offered by the SLM process has created a need for understanding how changes in the fabrication processing parameters affect the material structure, and in turn, how the produced structure affects the mechanical properties of the part. This study presents three different tools developed for the automated characterization of SLM 316L stainless steel (SS) material structures and the generation of realistic material structures for numerical simulation of mechanical performance. A defect content tool is presented to automatically identify and create binary segmentations of defects in SLM parts, consisting of small air pockets within the volume of the parts, from digital optical images. A machine learning based instance segmentation tool is also trained on a custom data set and used to measure the size of nanoscale cell features unique to 316L (SS) and some other metal alloys processed with SLM from scanning electron microscopy (SEM) images. Both these tools automate the laborious process of segmenting individual objects of interest from hundreds or thousands of images and are shown to have an accuracy very close to that of manually produced results from a human. The results are also used to analyze three different samples produced with different fabrication processing parameters which showed similar process-structure relationships with other studies. The SLM structure generation tool is developed to create melt pool structures similar to those seen in SLM parts from the successive melting and solidification of material from the laser scanning path. This structural feature is unique to AM processes such as SLM, and the example test cases investigated in this study shows that changes in the melt pool structure geometry have a measurable effect, slightly above 10% difference, on the stress and strain response of the material when a tensile load is applied. The melt pool structure generation tool can create complex geometries capable of varying spatially to create FGMs from a few user inputs, and when applied to existing simulation methods for SLM parts, offers improved estimates for the mechanical response of SLM parts.

Table of Contents

1	Introduction.....	1
1.1	Powder Bed Fusion and Selective Laser Melting	2
1.2	Functionally Graded Materials	6
1.3	Sample Characterization	6
1.3.1	Mechanical Testing.....	6
1.3.2	Sample Imaging	7
1.4	Computational Analysis	10
1.4.1	Process – Structure Relationships	10
1.4.2	Structure – Properties Relationships	12
2	Material Characterization.....	15
2.1	Sample Groups	15
2.2	Tensile Testing	16
2.3	Imaging Characterization	17
2.3.1	Material Prep.....	17
2.3.2	Defect Characterization Methods	18
2.3.3	Cell Structure Characterization Methods.....	21
2.4	Sample Characterization Results and Discussion	25
2.4.1	Mechanical Testing Results	25
2.4.2	Defect Characterization Results.....	26
2.4.3	Cell Characterization Results.....	30
2.4.4	Material Characterization Results Summary	38
3	Melt Pool Structure Computational Modeling.....	40
3.1	Introduction	40
3.2	Custom Melt Pool Structure Model	40
3.3	Modeling Methods	43
3.4	Test Cases.....	47
3.4.1	Comparison of Multiple Melt-Pool Geometries	47
3.4.2	Material Definitions from Test Data.....	52
3.4.3	Performance Prediction from Cell Geometry	55
3.5	Microstructure Modeling Results and Discussion	61
4	Conclusions and Future Work.....	63
4.1	Summary and Conclusions.....	63
4.2	Future Work	66
	References.....	67

List of Figures

Figure 1.1: Diagram of SLM machine and successive creation of melt pools [10]. Fair use determination under the Creative Commons Attribution License (https://creativecommons.org/licenses/by/3.0/).	3
Figure 1.2: SEM image of one of the samples created in this study showing a typical as printed 316L SS melt pool structure. One instance of the layer-layer and track-track MPBs are labeled.	4
Figure 1.3: SEM image of the melt pool and grain structure of one of the 316L SS samples produced here. The orange arrows show the preferential growth direction of some of the grains, with some grains forming at MPBs and others spreading across MPBs.....	5
Figure 1.4: Example image labels from the COCO data set showing a) image classification, b) object localization, c) semantic segmentation and d) instance segmentation. These are the ground truth annotations for this image and represent the desired outputs from an image processing model [33]. Used with permission from Springer Nature.	9
Figure 1.5: Example results from the modeling of grain growth in SLM AlSi10Mg according to the CET criteria [19]. Used with permission from Elsevier.	11
Figure 1.6: Molecular dynamics simulation result from Kurian and Mirzaeifar (2020) [18] showing expected microstructure morphology for a particular set of fabrication processing parameters. Used with permission from Elsevier.	12
Figure 1.7: Stochastically generated SLM grain structure based on the step-by-step packing method. Used for the simulation of deformation response [52]. Used with permission from Elsevier.	13
Figure 1.8: Example FEA structure of semi-circle melt pools and grains to simulate the deformation response of a SLM geometry using crystal plasticity [54]. Used with permission from Elsevier.	14
Figure 2.1: Representation of the dog-bone sample build strategy. A single laser scanning path aligned with the x direction was used throughout the part. The lines running in the y direction along the long axis of the part are representative of multiple build layers. The coordinat directions defined here are used throughout this study.....	16
Figure 2.2: Diagram, in mm, of the tensile test specimen machined from the as-manufactured SLM parts.....	16
Figure 2.3: Grayscale optical images at 20X magnification of the prepared a) group 2 sample showing the head on view of the melt pools from the x direction and b) group 1 sample showing the top view of the melt pools from the z direction. The complex grain structure can be seen as the contrasting lighter and darker regions within the image and the part defects can be seen as small dark specs often appearing near the melt pool boundaries.	17

Figure 2.4: SEM images of the prepped samples using image magnification ranging from 200x to 10,000x to observe the multi-level microstructural features. The images feature a) the melt pool structure and defects of the group 2 sample viewed along the x direction with a magnification of 200x, b) the melt pool structure and voids of group 3 in addition to some of the cellular features at a magnification of 500x viewed along the x direction, c) a few melt pools of the group 1 sample and some of the cellular structure clearly distinguishing different grains at 1,000x magnification and d) the cellular structure of the group 1 sample viewed from the z direction at a magnification of 10,000x. 18

Figure 2.5: Example raw optical image and processed binary image created using the custom Python script described above to identify voids in an optical image of sample group 1 viewed from the x direction. The original optical image is shown in a and the processed binary image is shown in b. Some of the black defect features are highlighted here with red circles to clearly show the defects detected by the script. 19

Figure 2.6: SEM images taken at 10,000x magnification to reveal the cell structure of the samples. Both images are viewing along the z direction and the specimens are from a) group 1 and b) group 3. 21

Figure 2.7: Screenshot of the online VGG Image Annotation tool used to define segmentation masks of each cell instance. Data is output in the JSON file format and used during the training and validation of the dataset. 23

Figure 2.8: Plot of some of the key training and validation statistics of the Mask R-CNN model used to evaluate the accuracy of the trained model's cell instance and segmentation predictions. All the loss values shown decrease with training and begin to converge at a lower value until the model begins to become over-fitted to the training data around step 27. 24

Figure 2.9: Engineering stress and engineering strain plot from experimental uniaxial quasi-static tensile tests of the sample specimens. Data recorded using DIC measurements and analysis. All samples were loaded to failure at a constant low strain rate. 25

Figure 2.10: Raw optical images of a) group 1, b) group 2 and c) group 3 samples showing some of the observed defects. 27

Figure 2.11: SEM images of highlighted defects from a) the group 2 sample viewed along the z direction at a magnification of 1,000x and b) the group 3 sample viewed along the x direction at a magnification of 2,000x. 27

Figure 2.12: Percent void content data measured by a custom Python script utilizing traditional image processing techniques on optical sample images. Histograms of the percent defect content measurements are plotted for sample group 1, 2 and 3 in a, b and c respectively. The mean and standard deviation of each sample group data set are shown. Fitted Weibull distributions of each data set are also shown and are plotted together in d for comparison. 28

Figure 2.13: Two example prediction outputs from the trained Mask R-CNN model showing the ability of the trained model to identify cell instances and produce segmentation masks with a relatively high degree of accuracy. Each segmentation mask is randomly colored, and a decimal number is given in the upper left corner of each instance bounding box to represent the classification confidence score from 0 to 1. Both

images are 512 by 512 px sections of different 10,000X magnification SEM images that were not included in the training or validations data sets. 31

Figure 2.14: Comparison of the red model predicted segmentation masks with the green annotated ground truth masks for four different 256 x 256 px images from the validation data set. The confidence and IOU scores are also shown for each detected cell. 32

Figure 2.15: Intersection over union (IOU) score distribution for all validation data set cell instances detected by the model. A best-fit Weibull distribution is plotted as a black line. 33

Figure 2.16: Comparison of measured cell area distributions from the validation data set calculated by the ground truth, green, and the model prediction, red, segmentation masks. Fitted normal distribution curves computed from the mean and standard deviation values for both data sets are also shown. The normal distribution was chosen rather than the Weibull distribution used for other results presented here because parameters for a well fit Weibull distribution were not found for these data sets. 34

Figure 2.17: Cell area data measured by the Mask R-CNN model from the SEM images are plotted for groups 1, 2 and 3 in a, b, and c respectively. The sample population average and standard deviation measurements are shown for each sample group. Fitted Weibull distributions are also plotted for each data set and shown together in d for comparison. 35

Figure 2.18: Primary dendrite arm spacing data distributions measured by the Mask R-CNN model segmentation predictions from the SEM images are plotted for groups 1, 2 and 3 in a, b, and c respectively. The average and standard deviation measurements are shown for each sample group. Best fit Weibull distributions for each data set are also shown and plotted together in d for comparison. 36

Figure 3.1: Section of example melt pool structure built by plotting unique intersecting parabolas. 41

Figure 3.2: Example melt-pool geometries created with custom melt pool generation tool to show some of the possible geometries and the effect of the user input parameters on the resulting geometry. 42

Figure 3.3: Example melt pool output showing a) the melt pool structure as seen in Abaqus for stress analysis, and b) the plot of the variation of user defined geometry parameters which define the morphology and distribution of the melt pools. 43

Figure 3.4: The same melt pool structure shown in Figure 3.3 is color coded to show each unique material definition a) in the melt pool structure and b) plotted according to the Ramberg-Osgood material response defined for each material. The engineering stress and engineering strain is plotted. 44

Figure 3.5: Example Abaqus geometry domain created with custom Python script. Periodic boundary conditions (PBC) are applied according to Eq. 3.4 and Eq. 3.5 below to create a representative volume element of the melt pool structure. The mesh nodes at the MPBs and apposing periodic edges are compatible. 45

Figure 3.6: A simple two material structure used to investigate the MPB geometry effects between stiff and soft materials. The melt pool structure with boundary conditions

and material definitions is shown in a along with the highlighted acute and obtuse angle MPBs. The Material 0 and Material 1 engineering stress vs engineering strain response is given in b.....	48
Figure 3.7: The a) stress and b) strain fields of the test case one melt pool structure from Fig. 3.6 above loaded to 20% true strain in the x direction. Interesting local features of the stress and strain fields are highlighted.	49
Figure 3.8: The a) stress and b) strain fields of the test case 1 melt pool structure shown in Fig. 3.6 above loaded in the y direction to 20% true strain. Interesting results near the lower layer-layer MPB are highlighted.....	49
Figure 3.9: The a) stress and b) strain fields of the test case 2 melt pool structure shown in Fig. 3.6 above loaded in the x direction to 20% true strain. Interesting results near the dissimilar material interfaces are highlighted.	50
Figure 3.10: The a) stress and b) strain fields of the test case 2 melt pool structure shown in Fig. 3.6 above loaded in the y direction to 20% true strain. The areas of maximum stress in each material are highlighted.	50
Figure 3.11: Plot showing the volume averaged effective engineering stress vs engineering strain response of all four test cases of the melt pool structure shown in Fig. 3.6. The engineering stress vs engineering strain responses of Material 0 and Material 1 are also plotted for reference.....	51
Figure 3.12: a) Melt pool structure with geometry and b) tensile engineering stress vs engineering strain response of the prepared dog bone samples measured with DIC. Material 0, 1 and 2 represent sample groups 2, 3 and 1 respectively.	52
Figure 3.13: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.12 above loaded in the x direction to 30% true strain. The areas of maximum stress are highlighted.	53
Figure 3.14: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.12 above loaded in the y direction to 30% true strain. The areas of maximum stress are highlighted.	54
Figure 3.15: Plot of the volume averaged effective engineering stress vs engineering strain response of the melt pool structure. Both the x and y direction results are plotted with the tensile responses of the three sample groups for reference.....	54
Figure 3.16: Process of converting a) section of raw SEM image to a b) a binary image separating the cell and cell boundary materials to be imported into Abaqus as a c) meshed geometry domain using a custom Python script.	56
Figure 3.17: Abaqus models of the sample group a) 1, b) 2 and c) 3 cellular structures imaged by SEM.....	56
Figure 3.18: The stress and strain fields of the a) group 1, b) group 2 and c) group 3 sample cell structures loaded to 10% true strain. Locations of local strain concentrations have been highlighted with red circles.....	57

Figure 3.19: The effective stress response of the cellular microstructures of the three sample groups is plotted along with the 316L and 4340 steel input material properties for reference.....	58
Figure 3.20: a) Gradient melt pool structure representing the observed melt-pool geometry found in the three different sample groups. This is the same structure as used above, shown in Fig. 3.12. b) The material definitions assigned to similarly colored layers of the melt pool structure, based on the results of the tested cell structures.....	59
Figure 3.21: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.20 above loaded in the x direction to 8% true strain.....	60
Figure 3.22: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.20 above loaded in the y direction to 8% true strain.....	60

List of Tables

Table 2.1: Fabrication processing parameters used for the three unique dog-bone sample groups.....	15
Table 2.2: Tabulated values of the average and standard deviation of the ultimate tensile strength and elongation at failure measured from the experimental tensile tests.	26
Table 2.3: Tabulated summary of some of the defect metrics for each sample group. The image defect content is the percentage of pixels representing a defect compared to the total number of image pixels and is also shown plotted in the histograms of Fig. 2.10 above. The defect area measurement is the area in square microns of each defect detected by the custom Python script. The defect count is an area-normalized measure of the average number of individual defects per square mm for each sample group.....	29
Table 2.4: Summary of the mean and standard deviation values for the cell area measurements calculated from the ground truth and model prediction segmentation masks.....	35
Table 2.5: Summary of the cell area measurements for the three sample groups, showing the average and standard deviation measurement statistics.	36
Table 2.6: Summary of the mean and standard deviation values for the primary dendrite arm spacing (PDAS) measurements of each group.	37
Table 3.1: User selected Ramberg-Osgood material properties defining the three materials.....	45
Table 3.2: Summary of the test conditions used in the FEA examples in the following sections.....	47
Table 3.3: The measured elastic modulus and yield stress of the example melt pool structure for both the x and y-direction test cases. The results of the rule of mixtures estimated elastic modulus is also shown with the percent difference comparison to the measured value.....	51
Table 3.4: Volume averaged effective elastic modulus and yield strength measured for both tensile loading conditions. The rule of mixtures estimated modulus and its comparison to the measured values are also given.	55
Table 3.5: Volume averaged effective elastic modulus and yield strength measured for each sample group cellular structure. The percent area composition of the stiffer 4340 steel is also shown for comparison.	59

List of Abbreviations

AM	Additive Manufacturing
SLM	Selective Laser Melting
FGM	Functionally Graded Material
FEA	Finite Element Analysis
316L SS	316L Stainless Steel
PBF	Powder Bed Fusion
SEM	Scanning Electron Microscopy
MPB	Melt Pool Boundary
PBC	Periodic Boundary Conditions
CM	Conventionally Manufactured
ASTM	American Society for Testing and Materials
CET	Columnar Equiaxed Transition
ROM	Rule of Mixtures
DIC	Digital Image Correlation
PDAS	Primary Dendrite Arm Spacing
COCO	Common Objects in Context
AI	Artificial Intelligence
CNN	Convolution Neural Network
CA	Cellular Automata
MD	Molecular Dynamics
VED	Volumetric Energy Density
RVE	Representative Volume Element
XCT	X-ray Computed Tomography
IOU	Intersection Over Union

1 Introduction

The 316L Stainless Steel (SS) selected for investigation here is a metal alloy very commonly chosen for additive manufacturing (AM) applications due to its favorable mechanical properties and printability. Additively manufactured 316L SS tends to have higher ultimate tensile strength and toughness compared to the conventionally manufactured material due to the unique microstructure developed during AM [1]. The advantages of great corrosion resistance and favorable machinability and weldability also contribute to make 316L SS a popular material choice in many fields such as nuclear energy, medicine, and aerospace [2]. The selective laser melting (SLM) AM process is one of the most popular AM technologies due to the high resolution and final part consistency and is the primary AM technique studied here.

Currently, AM 316L SS and many other AM materials present challenges in manufacturing which negatively impact the mechanical performance of the parts. To name only a few general challenges; AM parts often suffer from high residual stress build-up during manufacturing, causing excessive deformation or print failure. Insufficient powder melting and solidification leads to the formation of voids, generally referred to as defects, within the volume of the part. The AM parts are also often very sensitive to changes in the processing parameters used during manufacturing. A better understanding of the SLM AM fabrication process parameter selection and expected material properties are required to reliably manufacture AM parts and promote the adoption of AM in more industries and applications [3]–[5].

To address the challenges above, it is proposed in this study that the methods for SLM part microstructure characterization and prediction of part mechanical performance via virtual testing need to be improved. The improvements to the areas of material characterization and virtual testing should utilize and build upon existing techniques and technologies which have shown high accuracy results and should be as accessible as possible to facilitate increased data acquisition. The solutions developed here should be easy to use and fit into workflows used in other studies to maximize adoptability of these solutions. The accuracy of the solutions provided here should also match or be higher than that of the currently used techniques.

Current methods for material microstructure analysis produce high resolution and high accuracy results adequate for part characterization, but these methods often produce qualitative data which is challenging to compare between samples, especially samples from different studies. The equipment required for microstructure analysis is also often very expensive and complex, requiring skilled operators to collect data which limits the volume of data acquisition. Current simulation methods used to virtually test SLM parts and predict the mechanical performance have recently shown great accuracy with experimental results, but still feature many simplifications required to reduce the computational complexity. The simplifications limit some of the simulation accuracy and limit the range of produced AM part structures capable of virtually testing.

To improve the data analysis for AM part characterization, two unique tools are proposed here to reliably automate the characterization of defects and nano-scale cell features commonly present in 316L SS AM parts. Both features have been analyzed in numerous previous studies to characterize AM parts, but the manual identification and segmentation of these features from images is very time consuming and tedious. The goal

for the tools developed here is to fully automate the image analysis process using existing computer vision techniques to provide defect and cell feature segmentation data quickly and easily for quantitative part characterization. The microstructure feature segmentation predictions should be within about 10% error of manually produced segmentations to match the accuracy of traditional manual annotations. While evaluating the accuracy of the developed microstructure characterization tools, three sample groups of SLM 316L SS manufactured with different fabrication processing parameters are analyzed to compare the relationship between fabrication processing parameters and the expected defect content and cell morphology.

The destructive testing required to characterize the mechanical performance of AM parts can be costly in terms of time and resource requirements. Whenever possible, it is desired to simulate part performance via finite element analysis (FEA). Many of the FEA methods used in previous studies focus on estimating the material microstructure from fabrication process parameter inputs or the mechanical performance from the material microstructure features. The structure-performance estimations often rely on simplified semi-circle melt-pool geometries with included grain structures and sophisticated material models to estimate crack propagation and the localized material strain response. In this study, a melt pool structure generation tool is developed to provide more physically accurate melt-pool geometries of AM parts to improve upon the simplified semi-circle melt pools often used in other studies. The goal of the melt pool structure generation tool is to allow the creation of unique melt pool structures that are representative of observed manufactured samples. It is also desired that the melt-pool geometry be controllable by the user to easily achieve a desired melt-pool morphology. The effect of changing the melt-pool geometry is investigated in three example test cases of a functionally graded structure with periodic boundary conditions (PBC) under tensile loading. It is expected that the changes in the melt pool structure geometry will have a measurable effect on the local stress concentrations, especially near the interface between dissimilar materials, and will possibly also cause a measurable change in the volume averaged stress response of the structure.

Some of the current research dealing with the characterization and virtual testing of SLM 316L SS as well as relevant image processing techniques are reviewed below in section 1. The development of the image-based characterization and melt pool structure generation tools are presented in section 2. The accuracy of the characterization tools is discussed, and example analysis is performed on SLM 316L SS samples produced by three different sets of fabrication processing parameters. The development of the melt pool structure generation tool and three different quasi-static tensile tests are performed on geometries produced by the melt pool generation tool using FEA in section 3. Finally, section 4 summarizes the presented work with some of the key findings, conclusions and recommendations for future work.

1.1 Powder Bed Fusion and Selective Laser Melting

The selective laser melting (SLM) process is one of many different additive manufacturing (AM) techniques available capable of creating complex 3-dimensional metallic components. The SLM process utilizes a layer-by-layer production method in which local heat input via a laser scanning system can be controlled to solidify powdered

material into a desired part. The resulting part can then be post processed or used “as printed” depending on the application requirements.

The parts manufactured with additive techniques are not geometrically limited by conventional manufacturing (CM) techniques such as machining, joining, forming and casting. AM parts allow for more optimized and complex geometries designed for the application requirements rather than manufacturing requirements. Some SLM part materials also exhibit properties different than that of their CM counterparts, which are beneficial for some applications. SLM manufactured 316L SS, in particular, often exhibits increased ultimate tensile strength and ductility compared to the CM material due to the unique microstructure developed during SLM and not present in the CM material [6].

Modern AM technologies and materials are extremely appealing to a large number of applications and industries, with the aerospace and biomedical industries particularly interested [3], [4], [7], [8]. However, one of the biggest factors limiting the widespread manufacturing of parts via AM is quality control. There is currently a large need to better qualify AM final products because these parts are extremely sensitive to fabrication processing parameters and manufacturing conditions which make manufacturing reliability and consistency more difficult [9] [8].

The SLM process is a subset of the powder bed fusion (PBF) process, which is one of seven types of additive manufacturing (AM) technologies defined by the American Society for Testing and Materials (ASTM). The diagrams in Fig. 1.1 below show the basic components of an SLM machine and how SLM parts are formed.

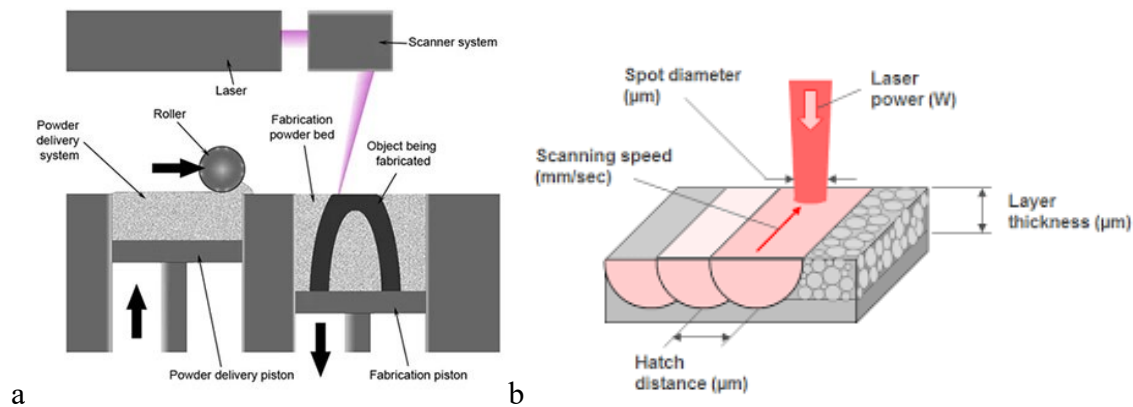


Figure 1.1: Diagram of SLM machine and successive creation of melt pools [10]. Fair use determination under the Creative Commons Attribution License (<https://creativecommons.org/licenses/by/3.0/>).

A SLM part is formed by successive melting and bonding of powder material via a scanning laser system. The part is created within the fabrication powder bed one layer at a time with an inert shield gas such as argon flowing across the build area to prevent oxidation [11]. Each layer of a part is fabricated by lowering the fabrication piston and spreading a layer of new powder over the part from the powder delivery system via the roller, also referred to as a recoater. The new layer of evenly spread powder is melted by the laser scanning system in the predefined locations and patterns to form the next layer of the solidified part. The fabrication piston then lowers to allow for a new layer of fresh powder, repeating the process until the full height of the part is complete.

The image in Fig. 1.1b shows a more detailed diagram of the powder melting and solidification during the SLM process as well as some of the key fabrication processing parameters which affect the resulting structure. In this example, a single laser scanning direction is used as indicated by the red arrow. The melt pools created by the laser are shown as pinkish semi-circles extruded along the laser scanning direction and indicate the material melted by each pass of the laser, very similar to the conventional welding process. Each new melt pool overlaps with some of the already solidified material within the previous melt pools in the same layer and in the layer below so that all of the melted material is fused into a single part.

The resulting melt pool structure of a SLM part is directly affected by the fabrication processing parameters chosen for manufacturing and influences the resulting mechanical properties. Experimental results show that melt pool boundaries (MPBs), especially track-track boundaries, tend to be the source of crack initiation and propagation in the tensile loading of SLM specimens, as well as one of the main reasons for the anisotropic behavior of SLM parts [12], [13]. Figure 1.2 below shows an as-printed melt pool structure with some of the track-track and layer-layer MPBs labeled.

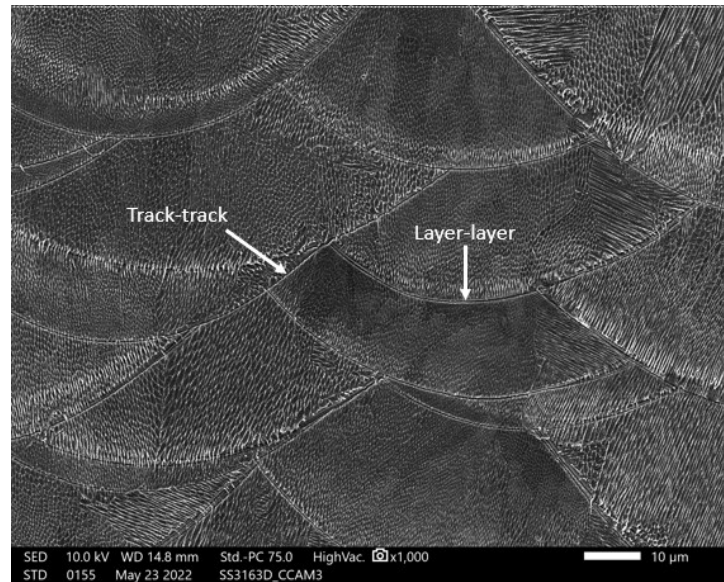


Figure 1.2: SEM image of one of the samples created in this study showing a typical as printed 316L SS melt pool structure. One instance of the layer-layer and track-track MPBs are labeled.

The SLM 316L SS alloy consists of metastable sub-granular cells, also referred to as nano-needles, pillars, columns and dendrites, as small as a few hundred nm in diameter, grain structures typically ranging from tens to hundreds of μm and melt pools which are typically hundreds of μm in size [14]. The highly localized heat input in the small melt pools creates large temperature gradients and cooling rates within the part, typically measuring greater than 10^6 K/s, which is much higher than cooling rates for conventional manufacturing (CM) processes, typically measuring 10^2 K/s and below [1]. The higher cooling rates create a complex cellular microstructure in addition to the melt pool structure and the typical grain structure, resulting in key features at multiple length scales [15].

The complete mechanics of cell structure formation are unknown, but the Constitutional Supercooling Theory and Interfacial Stability Theory can be used to

explain the unique solidification phenomena. The formation of cell structures are generally observed in a material system with binary alloys with specific solubility and melting point characteristics as described by Prashanth and Eckert (2017) [14]. Although 316L SS is not a binary alloy system, it acts as a two-phase system of an austenitic phase and other ferrite stabilizers. During solidification, the ferrite stabilizers are displaced from the liquid to form the cell boundaries rich in Mo, Cr and Si along the solid-liquid interface and the cellular structure is formed [14].

In addition to the formation of a cell structure in SLM 316L SS parts, the laser scanning path also creates a unique grain structure. Grain structures are also present in CM 316L SS, but the grain growth and therefore the resulting grain structure is unique for the SLM processed material. Much of the grain structure within SLM parts is dominated by epitaxial solidification and columnar grain growth. The grains tend to grow in the direction of the highest thermal gradient, which is perpendicular to the MPBs [16], [17]. Some of the grain growth directions within one of the samples created here are indicated below in Fig 1.3 by orange arrows.

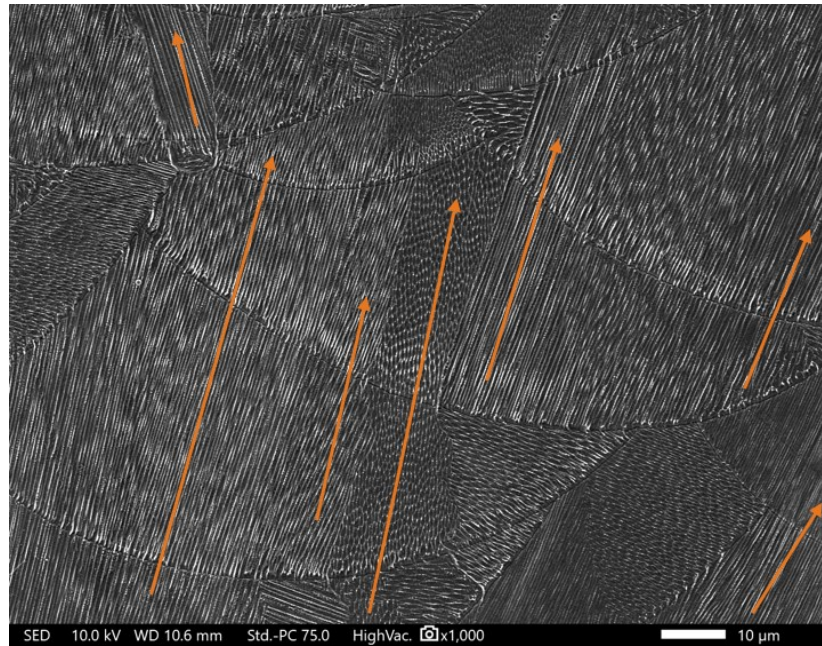


Figure 1.3: SEM image of the melt pool and grain structure of one of the 316L SS samples produced here. The orange arrows show the preferential growth direction of some of the grains, with some grains forming at MPBs and others spreading across MPBs.

The grain growth direction is predominantly pointing upwards along the z axis, or the build direction of the part, and mostly perpendicular to the MPBs, which contributes to the anisotropic properties of SLM parts. It is also observed that the same grain orientation is maintained across MPBs, indicated by areas of similar shading, which is characteristic of epitaxial solidification [18]. Although not observed in the image in Fig. 1.3, equiaxial grain growth is also expected in SLM parts according to the columnar to equiaxed transition (CET) prediction based on cooling and solidification rates controlled by fabrication process parameter selection [19], [20].

1.2 Functionally Graded Materials

Another unique advantage of the SLM process when compared with CM techniques is the ability to control the fabrication process parameters spatially throughout the part so that different fabrication processing parameters are used in different geometric locations of the part [17]. This is the fundamental method for creating a functionally graded material (FGM) in which certain properties of the material vary spatially. This is useful for applications in which the loading conditions for a given application are not uniform throughout the part. FGMs were initially developed as thermal barrier coatings for space applications, but these materials can also be found in nature in bone, teeth, wood and much more. Typical examples of manufactured FGMs are case-hardened metallic components such as shafts, bearing and gears in which the outer surface goes through a hardening process to reduce surface wear during service [21].

FGMs are similar to composite materials in that they combine different material properties in specific locations to achieve desirable part performance. However, one of the main advantages of FGMs over composites is that the property transitions are not as abrupt as in composite laminate materials for example. The relatively gradual transition of material properties helps to reduce the risk of failure at the composite material interface, a typical failure point [21], [22]. Similar to composite materials, the hardness of multi chemical composition FGMs was found to follow the rule of mixtures (ROM) according to the constituent properties [3].

1.3 Sample Characterization

The two primary characterization techniques used in this research to study the 316L SS SLM samples are tensile testing and microstructure imaging. Both characterization techniques help to relate the SLM fabrication processing parameters with the structure and performance properties of the samples. Archimedes' Principle volumetric density measurements are also conducted according to ASTM B962-17 [23] to compare with part density measurements obtained by sample imaging.

1.3.1 Mechanical Testing

The experimental tensile testing of small dog-bone specimens, 35 mm total in length, is performed on tensile test frames in which opposite ends of the specimens are gripped in the load frame and pulled apart. The tensile test is conducted in a load frame which measures the applied force to the specimen via a load cell attached in series with the specimen and the displacement of the sample is measured via the crosshead displacement of the load frame during testing. Especially when using small test specimens, the total force and displacement measurements are expected to be very small and thus susceptible to small measurement errors, especially for the measured displacement which can be affected by the deformation of the test frame. To overcome these measurement errors, the sample can be observed directly with a video camera to measure the local strain and estimate the local stresses at the surface of the specimen. This technique is called digital image correlation (DIC) and is widely used in component testing [24].

A random fine speckle pattern is applied to the specimen via a number of different methods so that the video camera has a clear view of many high contrast features. As the tensile displacement is applied to the specimen, the speckle pattern undergoes

deformation with the part, tracking the movement of the many high contrast features of the speckle pattern from one video frame to the next. The tracking of the local deformation of the speckle pattern allows for the local strain of the part to be estimated. Many software packages are available to perform the deformation tracking and computations automatically and there are many purpose-built cameras and lenses intended for DIC analysis, simplifying the process. Extensometers and strain gauges are also commonly used in specimen tensile testing to obtain accurate strain measurements, but unlike DIC, neither method measures local strains. Instead, extensometers and strain gauges measure the average strain within the gauge length of the sensor.

1.3.2 Sample Imaging

The material sciences have long relied on imaging methods utilizing a wide range of technologies of varying complexity to analyze the multi-level structural features of material samples [25]–[29]. Often the focus of the microstructure analysis is placed on extracting quantitative data to define process-structure-property relationships for a given material system [30]. Two of the frequently used imaging methods chosen to characterize material microstructure are optical and scanning electron microscopy (SEM) imaging. An optical microscope with a camera is used to observe features generally as small as tens of microns in size with good detail, while an SEM microscope is used to inspect nanoscale features, as small as a few nanometers, in high detail.

To view the microstructural features of the material, the surface of the sample is ground and polished to a mirror-like finish to remove the surface roughness which would otherwise dominate the features of interest. Etchants are also commonly used to reveal microstructural features because the etchant removes material by chemical reaction in different areas of the sample at different rates dependent upon the local material composition. The more eroded specimen areas form valleys in the surface of the sample which are easily detected by the imaging techniques above and perceived as lighter or darker features depending on their depth.

The primary features of interest in any material samples are generally manufacturing defects, the grain structure and any subgranular dendrite morphology, if present. The SLM 316L SS material studied here has a subgranular cellular structure characterized by columnar nano-needles often referred to as cells or dendrites [1]. The cell size is a measurement of interest which gives insight into the thermal development and solidification of the part, and with empirical trends the cell size can be used to estimate mechanical properties. The cell size is often measured as the primary dendrite arm spacing (PDAS), which is the Euclidean distance between the centroids of the two closest cell neighbors. The SLM 316L SS material studied here does not form secondary dendrite arms like some other materials, and therefore the PDAS measurement is directly related to the cross-sectional area of the cells. The measurements of both PDAS and cell area are presented in this study, but in general are herein referred to as cell size [31] [28].

Aiding in the visual analysis of microstructure images are several different software packages for general image analysis and materials science specific applications such as ImageJ, which offer tools to segment observed objects/features and produce quantitative metrics. The results are typically generated from segmentation masks, which are binary pixel masks of the features of interest that can be used to measure the feature morphology.

Traditionally, these segmentation masks are created by a researcher manually outlining each object of interest in each image. Manual object segmentation is a very time-consuming process, and the accuracy of the segmentation masks are dependent upon the care taken by the researcher to outline each object. Some modern image analysis tools allow for semi or fully automated feature segmentation using methods such as image thresholding and watershed segmentation. However, these image analysis and segmentation techniques have been shown by DeCost and Holm (2017) [32] to produce less accurate segmentation results for increasingly complex geometries. The features, such as color or edges, of an object need to be very distinguishable for most automated segmentation processes, and erroneous segmentations are more likely given more complex geometries. Instead, more sophisticated methods using computer vision and machine learning techniques are suggested by these authors for more accurate automated results. Currently available computer vision research has shown that accuracy within 10% difference between segmentation results produced by automated scripts and manual annotations is attainable and is used here to define segmentation results as accurate.

Recent advancements in the field of computer vision have greatly improved the identification and segmentation of features within images thanks to improvements in machine learning and computational power. These advancements often originate from the robotics and autonomous navigation fields, but the developed tools provide many interesting opportunities in many different research fields, including materials science.

A plethora of major computer vision advancements came following the release of the Microsoft Common Objects in Context (COCO) data set in 2015 [33]. The COCO data set provides computer vision researchers with over 200 thousand images with 1.5 million labeled object instances of nearly 100 different objects which are easily identifiable by an average 4-year-old. The availability of the COCO data set with high quality image labels, referred to as annotations, greatly reduced the barrier-to-entry for computer vision researchers, because the generation of annotated images for model training and validation is very labor intensive. This promoted a surge in computer vision object detection research with researchers working to produce improved artificial intelligence (AI) network architectures and models to score the highest object detection accuracy and speed, often referred to as the COCO Challenge. Some example outputs of interest in this field of study are depicted in Fig. 1.4 below for a random image from the COCO data set.

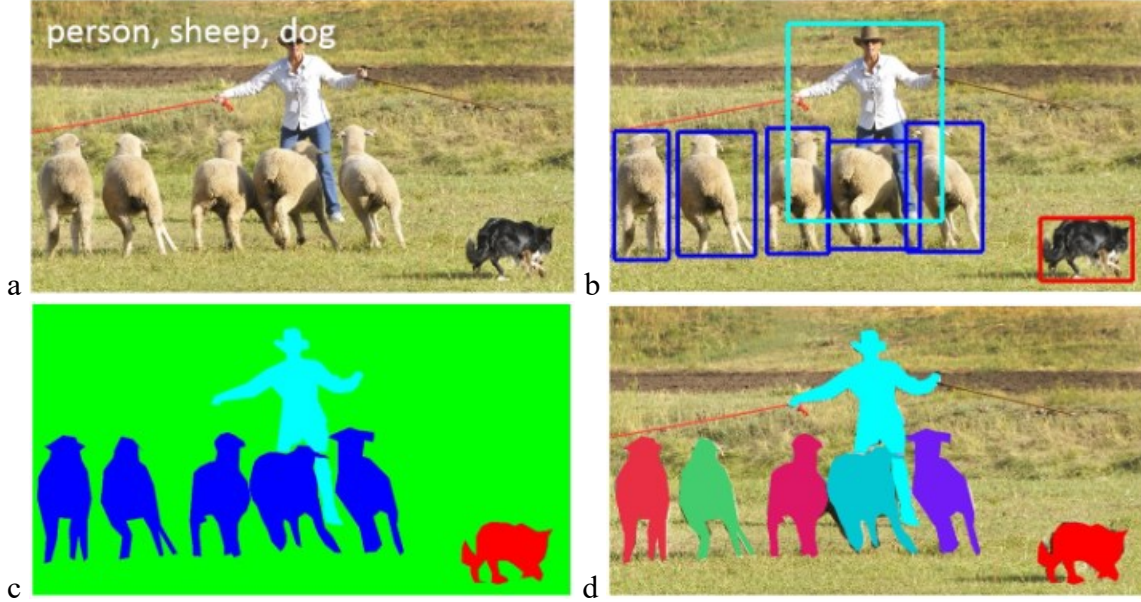


Figure 1.4: Example image labels from the COCO data set showing a) image classification, b) object localization, c) semantic segmentation and d) instance segmentation. These are the ground truth annotations for this image and represent the desired outputs from an image processing model [33]. Used with permission from Springer Nature.

Many of the newly developed computer vision object detection models rely on a convolution neural network (CNN) architecture [34], [35] which is designed to mimic the processes in the human brain responsible for object recognition. Recent CNN models have measured high object classification and segmentation accuracy for general objects, which has made CNNs desirable for the analysis of material microstructure images [29], [30], [32], [36].

The object recognition methods of most interest to material scientists are the semantic and instance segmentations shown in Fig. 1.4c and 1.4d but are also the most difficult of the methods presented [30], [29]. A particular CNN architecture of great interest is the mask region-based convolution neural network (Mask R-CNN) which achieved the highest score in the COCO instance segmentation challenge when released in 2017 by Facebook AI Research [34]. Mask R-CNN is an extension of Faster R-CNN [37], which measured good performance for object detection, with additional convolution layers for segmentation mask prediction and at the time of writing is regarded as the standard approach for instance segmentation [29].

Given large amounts of training data, Mask R-CNNs perform well in identifying objects within a training data set. Given an input image, a trained model can output a segmentation mask of the instance identifying which pixels within the image are occupied by the object. This can be done for any distinguishable object within the training data, making Mask R-CNN highly adaptable to nearly any object of interest.

Implementations of the Mask R-CNN architecture are open source and available online for anyone to use and modify, allowing Mask R-CNN to be applied to a wide range of vision processing and image analysis problems. A recent successful implementation of Mask R-CNN within the materials science field was used to measure particle size distribution and satellites in gas atomized metal powders [29].

The Mask R-CNN uses models, essentially large files composed of weights and connection definitions for the CNN, which are trained for the object(s) of interest to

produce the desired segmentations. Model training requires a large amount of labeled training data and is the process of changing model parameters to minimize the loss function shown in Eq. 1.1 using back propagation and stochastic gradient descent [29].

$$L = L_{cls} + L_{box} + L_{mask} \quad (1.1)$$

The loss L is defined as the sum of the classification loss L_{cls} , the bounding box loss L_{box} , and the segmentation mask loss L_{mask} . The term loss is analogous to the measured error between the annotated ground truth and model predicted value. A more comprehensive explanation of the model training process and other image segmentation methodologies used in the CNN are given by Cohn et al. (2021) [29] and others [30], [32], [34]–[36], [38], but is not described in detail here.

The amount of training data and training time required for the model to accurately predict segmentation masks for new objects can be reduced by using transfer learning and image augmentation. Transfer learning takes advantage of other models trained to identify many, nearly 100, different objects. These models have been trained with a large data set for a long period of time, which has produced highly optimized models for the segmentation of other objects. The additional training and optimization required to accurately segment an additional object newly added to the training data set is greatly reduced compared to the training required for a new model to produce similar accuracy results. Image augmentation is the process of altering images within the training data set, often by applying filters or some transformation, to improve model prediction accuracy. Image augmentation provides additional training images, the original plus augmented, and increases image variety, both of which yield higher model segmentation accuracy due to the higher number of different examples the model is exposed to during training.

1.4 Computational Analysis

The geometrically complex structures of SLM 316L SS ranging across multiple length scales makes creating useful computational models of significant size and detail capable of predicting microstructural feature formation during manufacturing and resulting mechanical properties difficult. Much of the current literature has focused on understanding the link between the fabrication processing parameters and the resulting material microstructure by examining the thermal evolution of the material. Presently, several studies provide models and explanations for some of the physical phenomenon effecting the microstructure development during the manufacturing of SLM 316L SS, but the cell structure formation is still not well understood. Recent attention has also focused on the structure-performance relationships between the observed material microstructure and mechanical performance of the parts. However, the complex hierarchical structures of SLM 316L SS make it difficult to estimate the macroscale material response. Both process-structure and structure-properties computational analysis methods are introduced in the following sections.

1.4.1 Process – Structure Relationships

Current works interested in the process-structure relationship of AM materials often focus on the thermal evolution and thermal history of melt pools via in-situ measurements and thermal fluid simulations [39]. These thermal fluid simulations are commonly used to provide insight into microstructure formation and defect content based

on selected fabrication processing parameters. Simulation of the thermal history of a SLM part is also very useful for predicting expected residual stresses and deformations when the part is separated from the build plate [40]–[43].

The melt pool structure is the primary length scale investigated in thermal fluid simulations because the melt pool is the size of the laser heat effected zone. Complex fluid flows caused by the Marangoni effect, intense thermal gradients, material vaporization and particle ejection are examined in the liquid melt pool. The predicted melt pool morphologies from the simulation results are often compared with in-situ melt pool morphology measurements for simulation validation. Accurate results have been reported by a number of authors for estimating the size of melt pools and estimating part deformation induced by thermal residual stresses [44]–[46].

Another important aspect of SLM part microstructure structure modeling is the solidification and growth of grains. Information from the thermal history of the part can be used to predict the grain growth using the CET criterion [19]. Columnar grain growth is typically seen at the melt pool edges where the thermal gradient is the highest and the surrounding material acts as a nucleation point for grain growth. Equiaxed grains are typically seen, if at all, near the center of the melt pools as shown in Fig. 1.5.

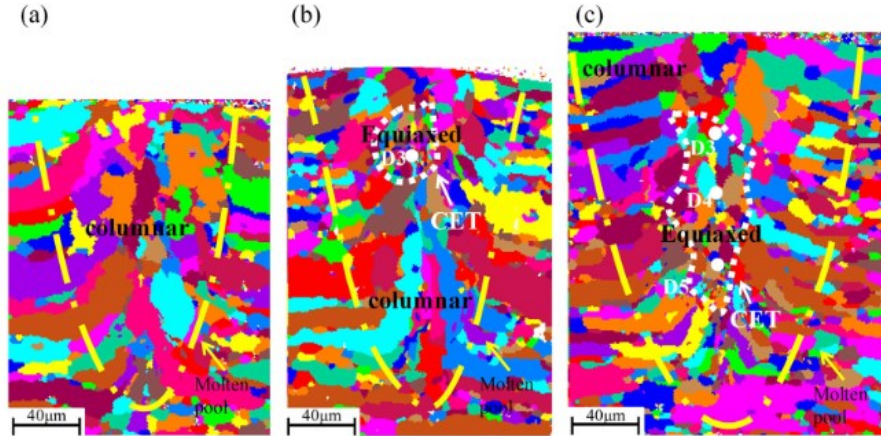


Figure 1.5: Example results from the modeling of grain growth in SLM AlSi10Mg according to the CET criteria [19].
Used with permission from Elsevier.

Other works such as that by Lopez-Botello et al. (2017) [47] uses a Cellular Automata (CA) model considering the heat flow characteristics from a coupled thermal FEA model to predict the grain growth from several melt pool tracks. The model produced good results, predicting many features of the resulting structure within about 15% error when compared to experimental measurements.

Smaller length scales of the SLM part structure are also investigated using different modeling techniques such as molecular dynamics (MD). One study in particular by Kurian and Mirzaeifar (2020) [18] investigated the SLM process on a nano scale to use MD to simulate the solidification and grain growth of nano particles melted via a scanning laser as shown in Fig. 1.6. The development of keyhole and lack of fusion voids were observed as expected for fabrication processing parameters yielding high and low volumetric energy densities (VED) respectively. The formation of columnar grains across MPBs also closely matched the physical structures observed from experiments.

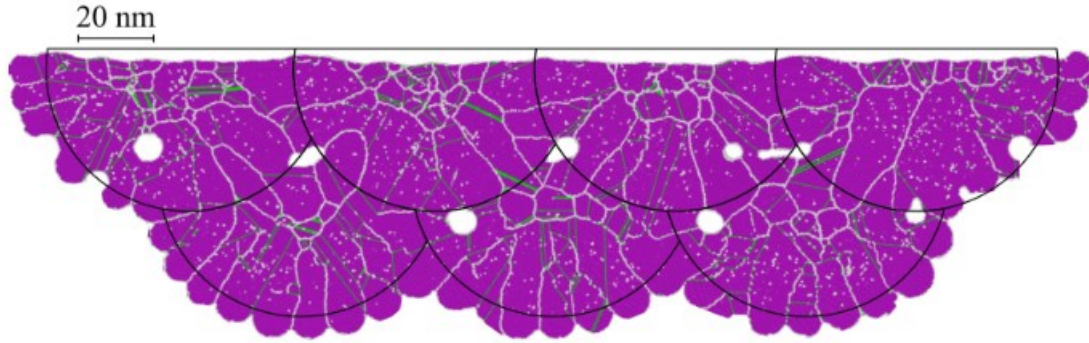


Figure 1.6: Molecular dynamics simulation result from Kurian and Mirzaeifar (2020) [18] showing expected microstructure morphology for a particular set of fabrication processing parameters. Used with permission from Elsevier.

Accurate modeling of melt pool structures allows manufacturers to make informed decisions about the fabrication process parameter selection to ensure successful prints and that the SLM parts meet the application requirements.

1.4.2 Structure – Properties Relationships

The connection between a material microstructure and expected mechanical properties is also valuable information for the manufacturing of SLM parts. With many works establishing models to estimate material microstructures based on fabrication processing parameters, relating the microstructure to the material properties allows for the direct prediction of material properties based on selected fabrication processing parameters in a virtual testing framework. Ideally, this would greatly reduce prototyping and experimental testing requirements for new SLM parts and allow for higher fidelity design adjustments. Some of the current work and modeling methods in this field are described below.

At the cellular nano scale of SLM 316L SS, results obtained by Kurian and Mirzaeifar (2020) [48] using MD to simulate the stress response of sections of a cell structure reveal a trend of increased yield and flow strength with increasing cell size. The MD methods used are similar to the nano SLM melt pool modeling studied by the same authors and provide accurate results at the expense of a small geometry domain and large computational requirements. The findings, however, disagree with the results of Agrawal et al. (2020) [31] who estimated SLM material yield strength from hardness measurements according to the Hall-Petch relationship. This discrepancy suggests that the Hall-Petch relationship may not be valid for estimating yield strength when considering cell size.

The cell geometry optimization FEA study conducted by Moneghan (2020) [49] suggested that the cell structure yield strength and tensile toughness measurements are highly dependent on the loading direction and load case. The cell geometries were optimized for a particular load case and loading direction at a time, and the findings showed that the optimized geometries were very different for each of the test cases. Optimization of the cell geometry for fatigue loading conducted by Ghodrati and Mirzaeifar (2020) [50] also suggests that the mechanical performance of SLM parts is highly dependent upon loading direction and cell morphology.

One of the difficulties with the simulation of SLM structures is the compromise between modeling complexity and physical accuracy. Generating custom structure

geometries manually is nearly impossible when trying to accurately represent physical examples. As a result, it is common in many studies to use a software solution for geometry creation. The model generation techniques are either based on measured samples or based on user inputs and meant to mimic realistic structures with some simplifications. The cell structure FEA analysis work flow developed by Moneghan et al. (2020) [51] is an example of a physically based structure geometry model. In Moneghan's work, an image processing framework is created to convert SEM images of cell structures into geometry to be imported into Abaqus for FEA. The resulting test geometry is nearly an exact duplicate of the imaged cell structure.

The user input derived models are often preferred to allow for experimentation with new structure geometries, but often lack detail in favor of simplicity. Many of the more sophisticated user input derived model generation methods involve some sort of stochastic seeding for features such as grains to mimic the nonuniform structure of SLM parts. An example of this approach is the step-by-step packing method used by Romanova et al (2021) [52] to create a 3-dimensional grain structure as shown in Fig. 1.7.

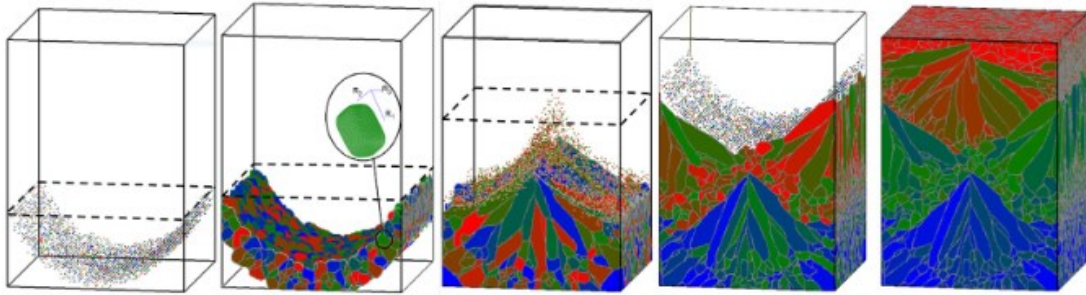


Figure 1.7: Stochastically generated SLM grain structure based on the step-by-step packing method. Used for the simulation of deformation response [52]. Used with permission from Elsevier.

However, even where a relatively complex method of grain growth approximation is used to mimic real SLM structures, other simplifications are often made to reduce the total complexity as seen by the semi-circular melt-pool geometries in Fig. 1.7.

Other relatively similar FEA studies aim to investigate the effect of grain size, defect content, material composition and more on the deformation response of 2-dimensional geometries containing about a dozen melt pools. In these studies [53]–[55], the geometry is kept relatively simple and instead the material models are developed to accurately predict the mechanical response of the parts. An example FEA structure from Ahmadi et al. (2016) [54] is shown in Fig. 1.8 below. A crystal plasticity model is used to model micro-scale deformation and a cohesive zone model is used at the MPBs to account for the local weakness in the structure. The grain structure is created by a stochastic Voronoi tessellation.

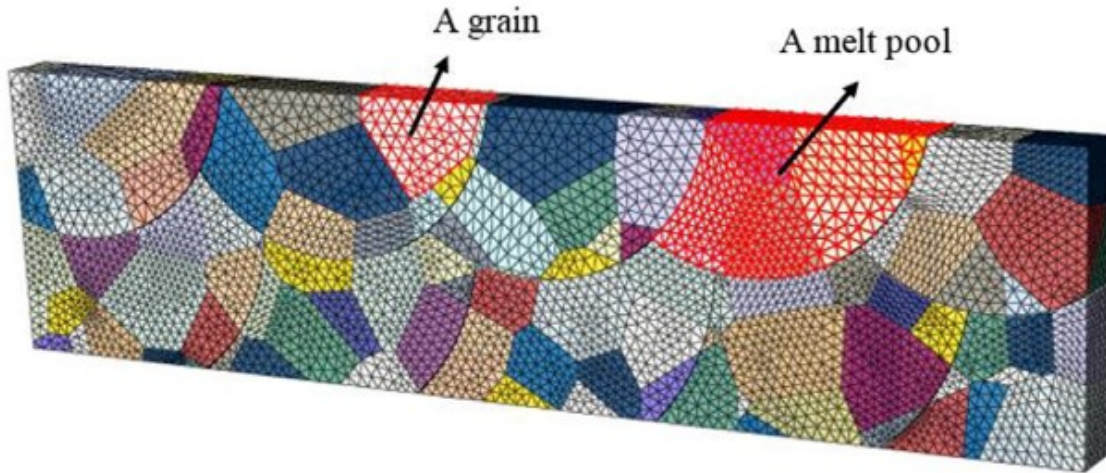


Figure 1.8: Example FEA structure of semi-circle melt pools and grains to simulate the deformation response of a SLM geometry using crystal plasticity [54]. Used with permission from Elsevier.

Other important considerations for the FEA models discussed here are the boundary conditions and the size of the test domain. In this case, the test domain is a representation of the total bulk structure, referred to as a representative volume element (RVE), and must contain a sufficient number of structure features to adequately represent the bulk structure [56]. For relatively simple repeating structures, the domain does not need to be very large. With added complexity and stochastic features, the size of the RVE will often need to be larger.

The assigned model boundary conditions can also have a large effect on the FEA results. The findings of van der Sluis et al. (2000) [57] showed that for the FEA of a RVE unit cell geometry and elasto-viscoplastic material, periodic boundary conditions (PBCs) were more accurate than uniform or mixed boundary conditions for repeating structures. The PBC is ideal for regularly repeating structures and can be applied to FEA models relatively easily following the procedure used by Akpoyomare et al. (2017) [58].

2 Material Characterization

2.1 Sample Groups

The 316L SS dog-bone samples analyzed in this study were manufactured with an EOS M 290 SLM printer [59] by the Commonwealth Center for Advanced Manufacturing using the fabrication processing parameters shown in Table 2.1 below. The fabrication processing parameters chosen for the dog-bone samples in Table 2.1 were varied slightly from the EOS recommended settings for 316L SS to study the effect of a range of parameters with slightly higher and lower volumetric energy density (VED) on the part microstructure.

Table 2.1: Fabrication processing parameters used for the three unique dog-bone sample groups.

Group	Laser Power (W)	Scan Speed (mm/s)	Hatch Spacing (mm)	Energy Density (J/mm ³)
1	225	1000	0.09	125
2	150	1100	0.075	90.91
3	175	1200	0.1	72.92

A constant layer height of 0.02 mm was used for each test group and was selected based on the average and maximum powder particle sizes used to manufacture the samples. The VED parameter shown is an estimate of the average energy per unit volume input into the part during processing. The VED is dependent upon the laser power, scan speed and hatch spacing parameter selections shown in Table 2.1 according to Eq. 2.1 below.

$$VED = \frac{P}{v * h * s} \quad (2.1)$$

The resultant VED is measured in units of J/mm³, the scan speed is represented by v in mm/s, the hatch spacing given as s in mm and the layer height represented as h in mm.

The dog-bone specimens were printed with a single direction laser path oriented along the thickness dimension of the part, as shown in Fig. 2.1 below. The scanning path direction was held constant for each printed layer and was chosen rather than a more typical multi-directional rotating scanning path so that all the melt pools in the final part align with the x direction of the part and are easily observable. This allows for easy viewing of all the melt pool cross section geometries from a single viewing direction without distortion and reduces the complexity of modeling the part by allowing a 2-dimensional microstructure geometry assumption.

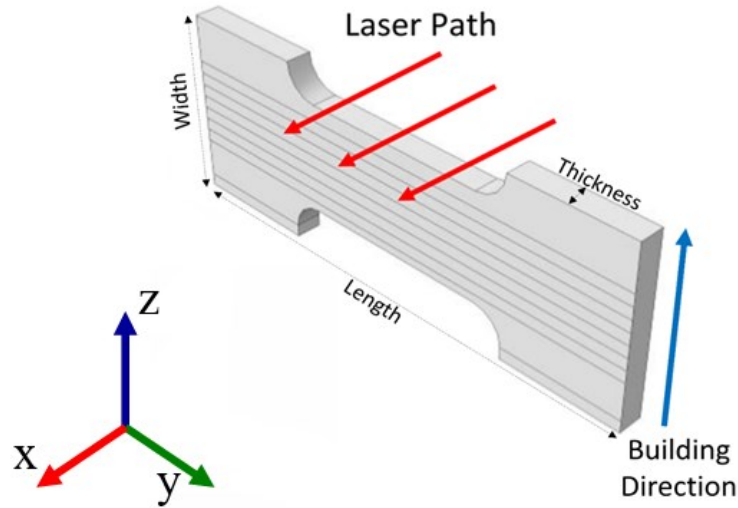


Figure 2.1: Representation of the dog-bone sample build strategy. A single laser scanning path aligned with the x direction was used throughout the part. The lines running in the y direction along the long axis of the part are representative of multiple build layers. The coordinial directions defined here are used throughout this study.

The dog-bone samples were cut away from the build plate via wire electrical discharge machining and machined to final dimensions measuring 35 mm in length, 10 mm wide and 2 mm thick with a gauge section of 7.5 mm long and 2.5 mm wide.

2.2 Tensile Testing

The specimens used for tensile testing were machined to a milled finish from the slightly over-sized as-manufactured SLM parts according to the dimensioned diagram shown in Fig. 2.2 below.

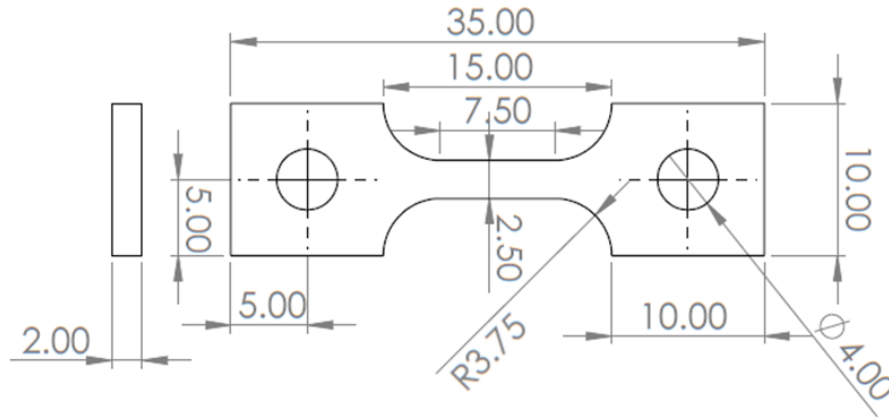


Figure 2.2: Diagram, in mm, of the tensile test specimen machined from the as-manufactured SLM parts.

A quasi-static tensile test was performed on each test sample one at a time by applying a constant strain rate until part failure. The test specimens were held in the Instron load frame using standard wedge action tensile grips. A speckle pattern was applied to the gauge section of the test specimen using a small airbrush for DIC analysis of the material strain. Three specimens from each group were tested for a total of nine

tensile tests. The resulting stress vs. strain plots for each test are given in section 2.4.1 below.

2.3 Imaging Characterization

2.3.1 Material Prep

Optical and Scanning Electron Microscopy (SEM) imaging was used to characterize the microstructural features of the samples produced via SLM. The main features of interest are the material melt pools around $150\text{ }\mu\text{m}$ in size, manufacturing defects about $6\text{ }\mu\text{m}$ in diameter and sub-granular cells which are about $0.4\text{ }\mu\text{m}$ in diameter. Optical imaging is used to analyze the manufacturing defects in the polished sample surface because it provides good contrast to observe the defects from the sample surface and adequate magnification. SEM imaging is used to observe the melt pools and the cells because SEM provides higher resolution and magnification compared to optical imaging for imaging smaller features.

To prep the samples for imaging, a tensile test specimen from each test group was cut into three pieces and fixed into a mount so that the material could be observed along each of the x, y, and z directions. The mounted samples were ground using a METPREP 3 Polishing/Grinding System with progressively finer grinding pads of 240 to 1200 grit. The samples were polished with a $6\text{ }\mu\text{m}$ glycol-based polycrystalline diamond suspension lubricant and finally with a $0.5\text{ }\mu\text{m}$ colloidal silica suspension lubricant. The prepped surfaces were then etched with a solution of nitrohydrochloric acid referred to as aqua regia to reveal the microstructural features [2]. The optical images used for defect analysis were captured before applying the etchant so that only the material defects are visible, because the etchant is not required to observe the defects.

Optical images such as those shown in Fig. 2.3 were taken to observe the grain structure, manufacturing defects and melt pool characteristics of the samples.

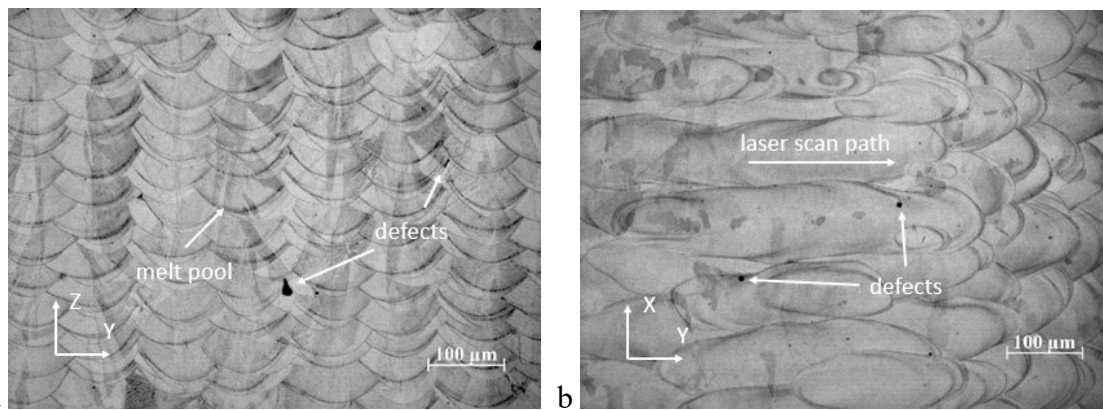


Figure 2.3: Grayscale optical images at 20X magnification of the prepared a) group 2 sample showing the head on view of the melt pools from the x direction and b) group 1 sample showing the top view of the melt pools from the z direction. The complex grain structure can be seen as the contrasting lighter and darker regions within the image and the part defects can be seen as small dark specs often appearing near the melt pool boundaries.

The images taken from the x direction show the height and width of the melt pools, while the images from the y and z directions show the side and top views of the melt pools respectively.

In addition to the melt pool and grain structure, the sub-granular cell structures are also visible via SEM imaging of the same samples at a much larger range of magnification levels. Figure 2.4 below shows a variety of SEM images revealing some of the features of the SLM part microstructure.

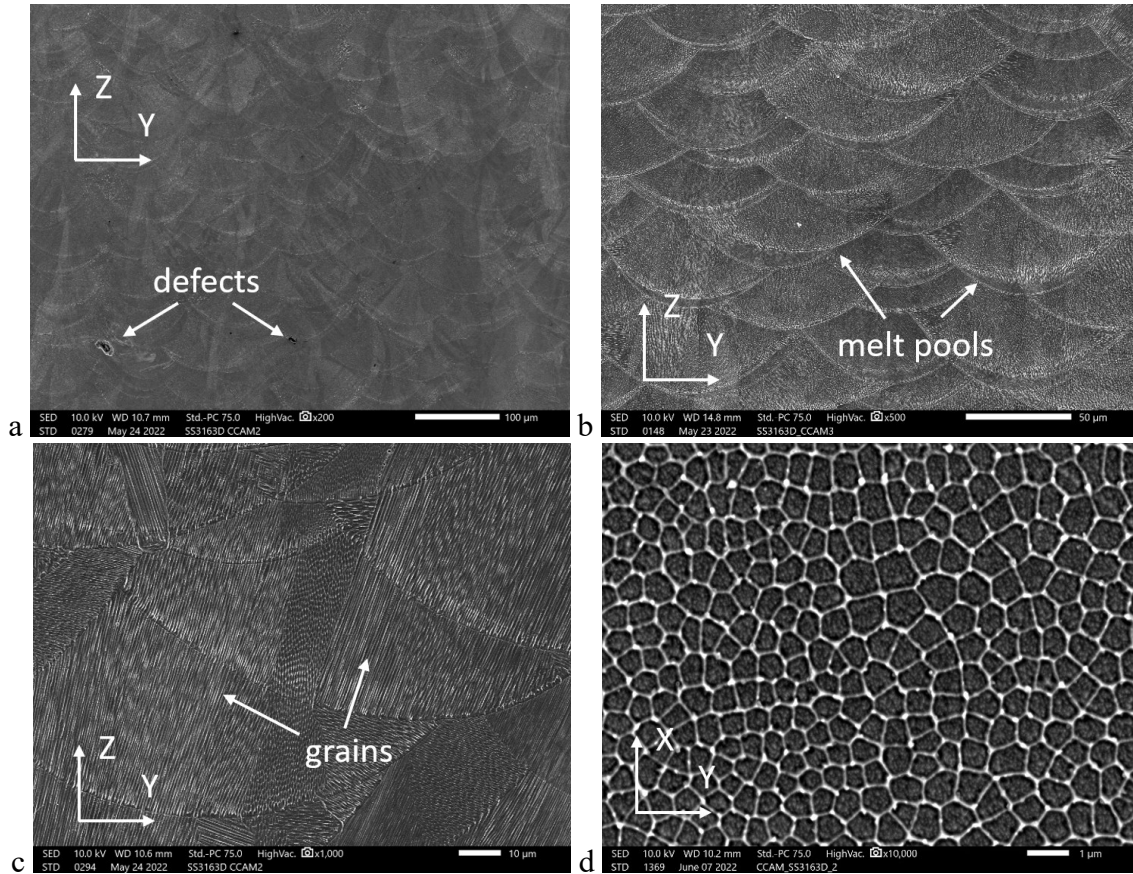


Figure 2.4: SEM images of the prepped samples using image magnification ranging from 200x to 10,000x to observe the multi-level microstructural features. The images feature a) the melt pool structure and defects of the group 2 sample viewed along the x direction with a magnification of 200x, b) the melt pool structure and voids of group 3 in addition to some of the cellular features at a magnification of 500x viewed along the x direction, c) a few melt pools of the group 1 sample and some of the cellular structure clearly distinguishing different grains at 1,000x magnification and d) the cellular structure of the group 1 sample viewed from the z direction at a magnification of 10,000x.

The clearly observable microstructure from both the optical and SEM images indicates that the material polishing and etching was successful. The resulting images are ideal for qualitative structure characterization and quantitative characterization of the part defects and cell sizes according to the methods described below in sections 2.3.2 and 2.3.3.

2.3.2 Defect Characterization Methods

Using traditional image processing methods, a large collection of about 450 1292 x 968 px optical images of the three sample groups before etching were analyzed to

quantitatively measure the defect content of the SLM manufactured parts. A custom Python script was developed to create binary segmentation masks of defects within the captured optical images and to return quantitative metrics for the percent defect content, number of defects and defect size distribution for each sample group.

Optical images of each prepped sample were methodically captured in a grid pattern to minimize overlap and gaps between images so that nearly the entire prepped surface of each sample was imaged. The surface area captured by each image measures 0.365mm^2 , and from the roughly 150 x, y, and z-oriented images of each sample, about 55mm^2 of prepped surface area was captured to represent each of the three sample groups. A custom Python script utilizing the OpenCV computer vision processing library, a widely used image manipulation resource with capabilities like those of the popular ImageJ software, was used to segment manufacturing defects for characterization. The primary benefit of using the OpenCV Python library rather than ImageJ is that the image segmentation and analysis procedure as well as the data post processing can be automated very easily all within the Python environment.

To create segmented binary images from the raw grayscale optical images, such as the image shown in Fig. 2.5a below, the images are first converted from a three-channel color format to a single channel 8-bit grayscale image. A bilateral filter is applied to smooth image features and reduce the amount of noise in the images while preserving feature edges. The mode is then calculated from the distribution of color values measured from each image. The mode of the color values of a single image corresponds to the grayscale color value of the prepped surface free of any defects. A binary threshold operation is performed on each unique image using a threshold color value slightly darker than the mode to create the binary image shown in Fig. 2.5b. The defects are now clearly defined as black pixels in a binary image and can easily be analyzed to obtain several different quantitative measurements. The defect metric of most interest is the percent defect content of the part and is measured here by counting the total number of black pixels representing voids.

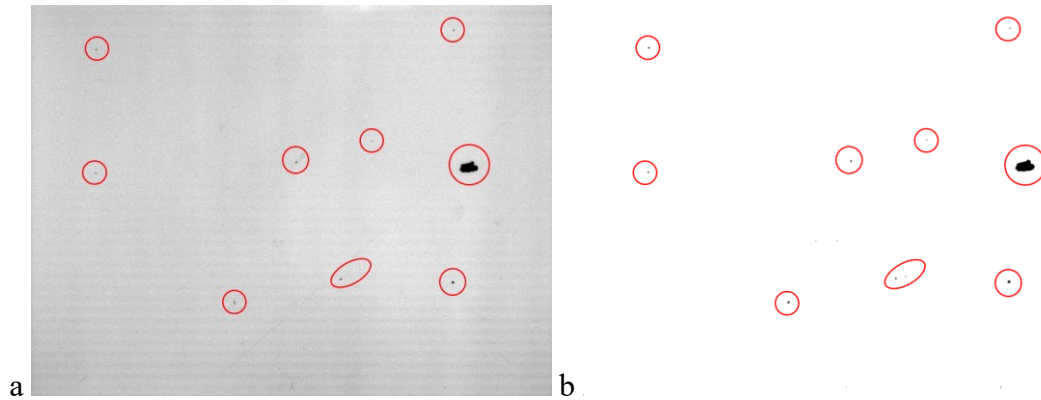


Figure 2.5: Example raw optical image and processed binary image created using the custom Python script described above to identify voids in an optical image of sample group 1 viewed from the x direction. The original optical image is shown in a and the processed binary image is shown in b. Some of the black defect features are highlighted here with red circles to clearly show the defects detected by the script.

Selecting the threshold value based on the mode of the measured color values of each image ensures that, even for a range of raw optical images and image settings, the Python script can determine the unique color value representing the background and

correctly isolate the darker defect features from the bulk material. A threshold value about 40 units darker than the mode was used for each image to ensure features not of interest, such as shadows, were not incorrectly segmented as defects. Near this threshold value, the final void content measurements were insensitive to small changes in threshold value, indicating that the script is capable of reliably segmenting defects from optical sample images while ignoring other features not of interest.

With the binary segmented images, the total number of black pixels representing defects is totaled and compared to the total number of pixels in the image to measure the percent defect content for a given image. To analyze individual defects, a Canny edge detector operation is applied to the binary image, such as that shown in Fig. 2.5b, to identify each of the void edges. By identifying each fully enclosed defect edge, each void instance can be identified and segmented. The Canny operation is expected to produce accurate void instance segmentation masks because it is performed on binary images, which have clearly defined feature edges. At this point each void can now be referenced independently, providing a measurement of the number of individual voids in an image, and a measurement of the area of each individual void.

The part density of each sample group was also measured using the Archimedes' Principle according to ASTM B962-17 [23]. This volumetric density-based porosity measurement provides a density measurement for an entire part based on mass measurements. The density measurements are compared with the image processed defect measurements to test the accuracy of the image-based defect measurements. The results of the defect analysis for the SLM samples produced here are given in section 2.4.2 below.

In some cases, scratches were visible on the polished and etched surface remaining from the material surface prep process and were erroneously identified as manufacturing defects. To remove the unwanted scratches from the defect results, the length and width of each individual defect was measured by creating a rotated rectangular bounding box circumscribed about the defect. The length and width measurements were used to calculate the slenderness ratio of each void, and the voids with a slenderness ratio greater than 10 were assumed to be scratches and removed from the data set.

Although the image processing methods used here to analyze the sample void contents are quite reliable and robust for a variety of similar input images, only a relatively small 2-dimensional section of the 3-dimensional part is sampled for measurement and characterization. The imaged surface is assumed to be representative of the entire thickness of the part so that the measured defect area directly correlates with the volumetric defect content of the sample. For each sample, the imaged surface is selected at a random depth far enough from the edges of the sample so that the bulk microstructure of the part is analyzed, but it does not measure the volumetric void content directly.

Image based 2-dimensional defect analysis techniques are suggested by Suryawanshi et al. (2017) [27] to be more accurate than the popular Archimedes' principle volumetric density measurements because unmelted powder entrapped in lack of fusion voids does not erroneously effect the imaged defect measurements as it does the part volumetric density measurement. The sample images also provide additional quantitative and qualitative information about the defect types, size distribution, and

morphology which are not provided by the Archimedes' principle volumetric density measurements.

Higher accuracy results can be attained using methods such as X-ray computed tomography (XCT), which can detect porosities and create a three-dimensional model of the imaged sample volume. XCT imaging techniques have been used by Liu et al. (2020) [25], Agrawal et al. (2020) [31] and others to image and analyze defects within the volume of the sample, but this method requires expensive specialized equipment. The XCT method is therefore less accessible, and the increased accuracy of the XCT results does not necessarily justify the additional cost and complexity.

2.3.3 Cell Structure Characterization Methods

A custom trained Mask R-CNN model is developed here to automate the microstructure image analysis of SLM 316L SS cells. Some of the SEM images of the three sample groups created here were annotated manually to define the cell geometries and used to train the Mask R-CNN model with the assistance of transfer learning and image augmentation. Some of the relevant model training statistics used to estimate the accuracy of the model are presented and predict relatively high model segmentation accuracy. The segmentation masks predicted by the Mask R-CNN model are used to measure the cell areas by counting the number of segmented pixels, and the PDAS by measuring the Euclidean distance between neighboring cell center points. These measurements provide cell size data useful for characterizing the cell structure.

The cell structures of the prepped samples were inspected using SEM imaging. The SEM images, such as those shown below in Fig. 2.6, have a dimension of 2560 x 2048 px and were taken at a magnification of 10,000x to observe the cellular structure features measuring about one micron and below in diameter.

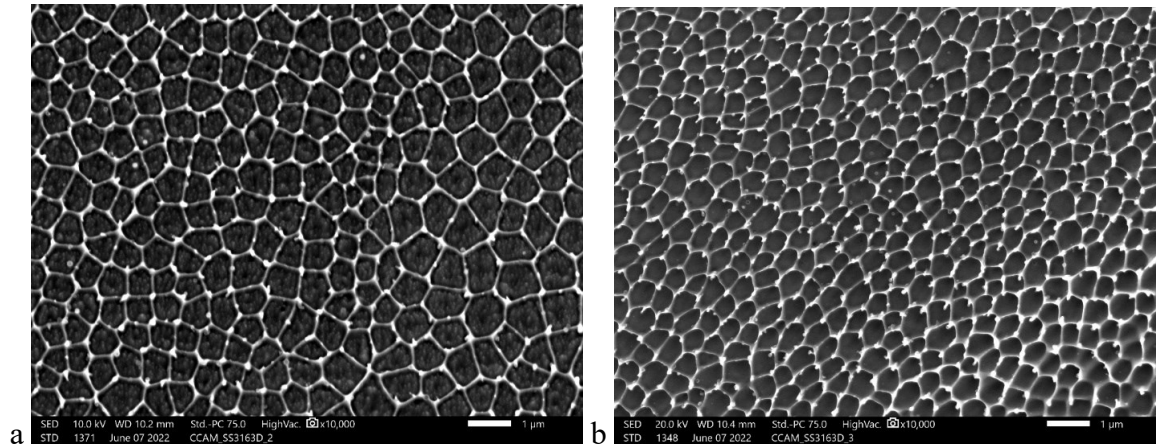


Figure 2.6: SEM images taken at 10,000x magnification to reveal the cell structure of the samples. Both images are viewing along the z direction and the specimens are from a) group 1 and b) group 3.

The SEM images used to represent the cell structure of each sample were taken viewing the sample from the z direction. Due to the thermal gradient created by the laser, the preferential growth direction of the material aligns with the z direction. Aligning the viewing orientation with the growth direction of the cells allows a larger amount of the nearly circular cell cross-sections to be observed head-on without distortion and elongation. Still, the cell growth direction does not align with the z direction perfectly

throughout the entire sample and only certain areas of the prepped surface where the cells were observed to align best with the z direction were selected for imaging.

The resulting images provide a detailed representation of the distribution of cell shape and size across the imaged area, and it is assumed that the imaged area is representative of the entire sample. To quantitatively measure the cell areas, a Mask R-CNN was trained to identify individual cell instances and used to characterize the cells in the images, similar to the methods utilized by Cohn et al. (2021) [29]. More specifically, an open-source implementation of Mask R-CNN, introduced by Facebook AI Research in 2017 [34], based on a Feature Pyramid Network and a ResNet 101 backbone using Python, Keras and Tensor Flow was used to create bounding boxes and segmentation masks for each detected cell instance [60]. The resulting segmentation mask for each cell feature, such as those shown in Fig. 2.6 below, is treated as a cell object and is used to characterize the cellular structure.

With the cell segmentation mask data, useful quantitative metrics such as the cell area and primary dendrite arm spacing (PDAS) can be measured very easily. Summing the number of pixels in a single cell segmentation mask and converting to μm^2 yields the measured cell area. Calculating the location of the geometric centroid for each cell segmentation mask in an image and measuring the minimum Euclidean distance between the neighboring centroids yields the PDAS. The results of the cell area and PDAS measurements are presented and discussed in section 2.4.3 below.

To train the Mask R-CNN model to accurately identify cell instances, 28 SEM images like those shown in Fig. 2.5 were taken of the three prepped 316L SS samples, each from a different test group. The 2560 x 2048 px images were divided into smaller 256 x 256 px images to create a total of 2240 images. The smaller images were used for model training to increase the number of images available for training and reduce the system memory requirements when processing each image. A random selection of 136 out of the 2240 images were annotated in the online VGG Image Annotation tool developed by Dutta and Zisserman (2019) [61] to create the training data set. The annotations of one of the 256 x 256 px images are shown below in Fig. 2.6. A smaller set of 35 images randomly selected from the 2104 remaining images not used in the training data set were annotated just like the images of the training data set to create the validation data set, which is used to estimate the accuracy of the model during and after training.

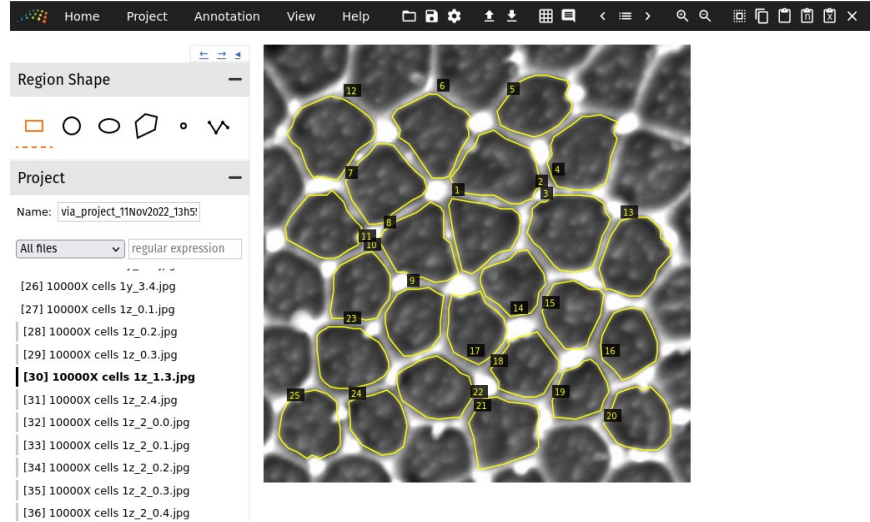


Figure 2.7: Screenshot of the online VGG Image Annotation tool used to define segmentation masks of each cell instance. Data is output in the JSON file format and used during the training and validation of the dataset.

The annotations define the ground truth segmentation mask of each cell instance in the image, and the process is nearly identical to manually segmenting the cells for characterization and data analysis within software such as ImageJ. However, instead of the annotations being useful for only a single image, the annotations are used to train the Mask R-CNN model to recognize and correctly segment cell instances in new images without any manual user processing. Cells which are near the edge of the image and only partially visible are not annotated. The area of cells not completely within the image boundary would be incorrectly measured as smaller than the true value. Therefore, it is desired that the trained model ignores cell instances which are not fully visible to increase the accuracy of the cell size measurements.

To improve model training results with the relatively small training data set, image augmentation was applied to the training images to diversify the training images and mimic a much larger training data set. The image augmentation used here is from an open source Python library developed by Jung et al. (2020) [62]. The specific image augmentation methods used on the training data set include a random selection and combination of several relatively small image adjustments selected to mimic possible raw SEM image variance. The augmentation methods used include adjustments to black and white levels, contrast, image orientation, image blur and image noise.

Using the 136 annotated images of the training data set with augmentation, the model was trained on a desktop computer with a dedicated graphics card to reduce computation time. The model was trained for a total of 40 steps, each with 1000 iterations, and the resulting model performance is discussed below and in section 2.4.3.

Some of the relevant model training loss statistics are plotted in Fig. 2.7 below, where all the loss metrics are given ranging from 0 to 1 with a lower value indicating higher accuracy. After about 27 steps, the validation loss and validation mask loss reach a minimum and then begin to increase while the loss and mask loss continue to decrease. The increase in the validation metrics and continued decrease in the training metrics suggest that the model is becoming over-fitted to the training data after about 27 training steps. Beyond the 27th training step the model is becoming less accurate in segmenting

cell instances from the validation data set, which are not present in the training data set, and will therefore likely be less accurate in segmenting cell instances in new images.

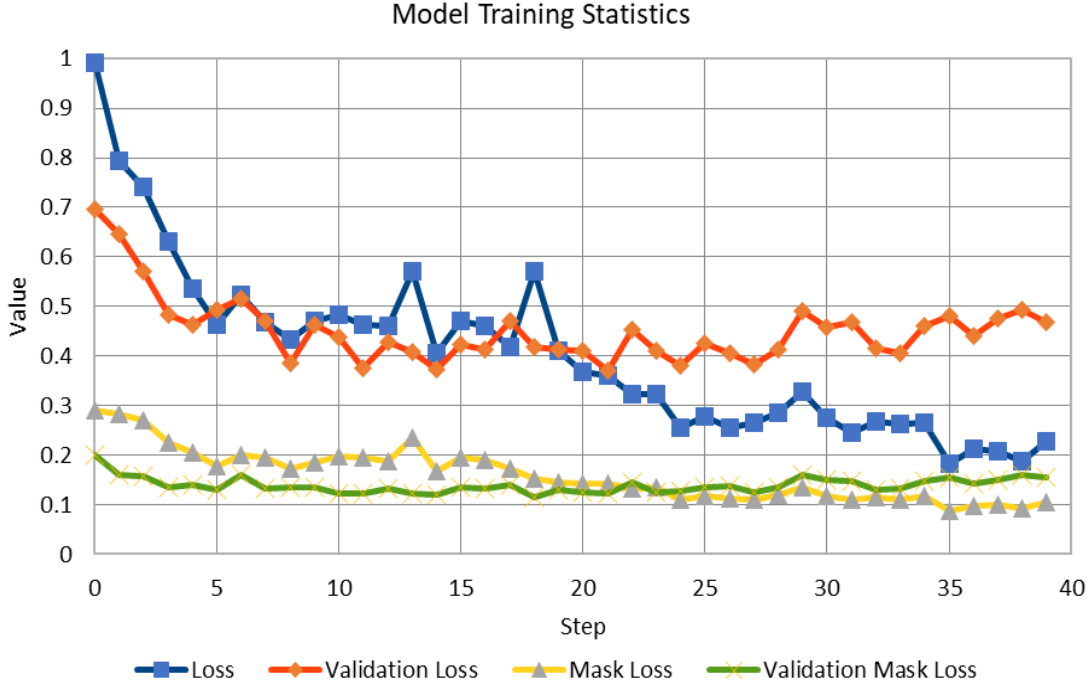


Figure 2.8: Plot of some of the key training and validation statistics of the Mask R-CNN model used to evaluate the accuracy of the trained model's cell instance and segmentation predictions. All the loss values shown decrease with training and begin to converge at a lower value until the model begins to become over-fitted to the training data around step 27.

The data over-fitting can be reduced or eliminated by including more annotated training data or by adjusting some of the model training parameters such as learning rate and initial weights. However, generating more annotated training data is quite labor intensive and tweaking model training parameters is expected to result in only a small possible improvement to the model accuracy. The validation mask loss statistics measured at the 27th training step suggested that the segmentation mask predictions by the model are about 85% accurate. This estimated accuracy was considered sufficient for the cell measurements here, and further work to increase accuracy would not be worth the additional effort. Therefore, the model created at the completion of step 27 was selected for all further image analysis.

To quantitatively assess the accuracy of the model, predicted segmentation masks were compared with the corresponding annotated ground truth segmentation masks of the validation data set using the intersection over union (IOU) measurement described by Cohn et al. (2021) [29] shown in Eq. 2.2 below.

$$IOU(A, B) = \frac{A \cap B}{A \cup B} \quad (2.2)$$

The numerator, $A \cap B$, is the number of pixels shared between segmentation masks A and B, and the denominator, $A \cup B$, is the total number of unique pixels in the segmentation

masks of A and B. The IOU score ranges from 0 to 1, with a value of 1 representing a perfect pixel-for-pixel match between the predicted and ground truth segmentation masks.

This metric was chosen to evaluate the model rather than the precision and recall scores commonly used to evaluate and compare instance segmentation models in projects such as the COCO challenge because the segmentation mask is the model output of most interest for the measurements here. The precision and recall scores are averaged across many instance classes, because most instance segmentation models are interested in identifying many different objects within a large data set of images with many classes. Unlike many instance segmentation models, the model developed here is trained to identify only a single cell class and it is not critical that every cell within an image is identified, just that the segmentation masks of the identified cells have a high accuracy.

The results of the cell image analysis and cell structure characterization using the trained model as well as further discussion on the accuracy of the model predictions and the cell size results are provided in section 2.4.3 below.

2.4 Sample Characterization Results and Discussion

2.4.1 Mechanical Testing Results

The engineering stress vs. engineering strain results from the tensile tests of the dog bone specimens are shown in Fig. 2.9 below. Three samples from each group were tested to failure and similar results are observed for each sample group.

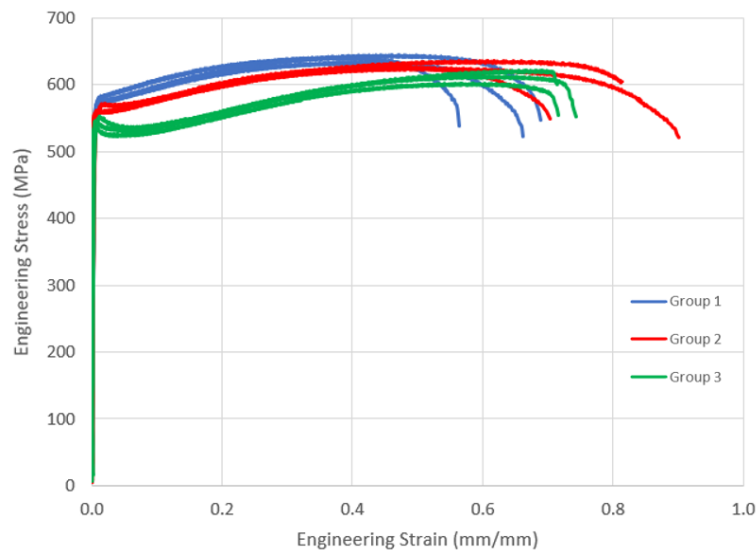


Figure 2.9: Engineering stress and engineering strain plot from experimental uniaxial quasi-static tensile tests of the sample specimens. Data recorded using DIC measurements and analysis. All samples were loaded to failure at a constant low strain rate.

The averages and standard deviations of the measured ultimate tensile strength and elongation at failure from the experimental tensile tests are shown in Table 2.2 below. Each test group measured a relatively high elongation at failure, as is expected with SLM 316L SS material. Sample group 2 measured the highest average elongation at failure, averaging just over 0.8 mm/mm, and group 1 the lowest, averaging slightly more

than 0.6 mm/mm. The group 1 samples measured the highest yield and ultimate tensile strength, and the group 3 samples the lowest. The ultimate tensile strength of each test group was relatively similar, with a total difference in average measurements of about 28 MPa between the three test groups. The group 1 average ultimate tensile strength measured the highest, at 640 MPa, and the group 3 average measured the lowest, at 612 MPa. The standard deviation in both the ultimate tensile strength and elongation at failure measurements are lower than the difference between the corresponding averages in ultimate tensile strength and elongation at failure measurements between test groups. This indicates that the changes in fabrication processing parameters between test groups have a significant effect on the mechanical properties of the samples.

Table 2.2: Tabulated values of the average and standard deviation of the ultimate tensile strength and elongation at failure measured from the experimental tensile tests.

Group	Ultimate Strength (Mpa)		Elongation at Failure (mm/mm)	
	Average	Standard Deviation	Average	Standard Deviation
1	640.35	5.05	0.639	0.066
2	629.56	5.91	0.807	0.098
3	612.56	9.74	0.725	0.017

In the measured stress vs strain curve of the group 2 and especially the group 3 samples, a unique dip in the measured stress is observed immediately after yielding of the material. This is commonly referred to as a yield point phenomenon and according to Koztowska et al. (2019) [63] is due to the formation and movement of Lüders bands, usually observed in low carbon steels but not frequently seen in SLM 316L SS.

Due to the very small strains in the elastic region of the tensile test, the DIC measured strain for each of the samples was relatively inaccurate. The data within the elastic region was manually linearized according to the yield point, estimated by locating the knee in the stress response curve, and the average recorded elastic slope. The measured difference in elastic modulus between each group was minimal, with the variance between samples of the same group nearly identical to the variance between groups.

2.4.2 Defect Characterization Results

A qualitative analysis of the optical images reveals that a combination of both keyhole and lack of fusion voids are present in each of the sample groups. Figure 2.10 below shows raw optical images for each sample group selected to represent the defect content of the corresponding group. The various void defects are clearly visible as small black specs in each of the images and the relative sizes and quantities can be compared.



Figure 2.10: Raw optical images of a) group 1, b) group 2 and c) group 3 samples showing some of the observed defects.

Visually, the group 1 sample image in Fig. 2.10a contains the fewest number of defects which are mostly small round keyhole voids similar to those seen in the group 3 sample image, Fig. 2.10c. The group 2 sample image in Fig. 2.10b contains the largest defects which are less round than the defects seen in the group 1 and 3 samples, suggesting that these are lack of fusion voids. The number of defects in the group 2 sample appears to be nearly equal to that of the group 3 sample. A closer inspection comparing the voids from the group 2 and 3 samples in the SEM images of Fig. 2.11 below supports that the group 2 sample is composed of lack of fusion voids and the smaller round defects found in the group 1 and 3 samples are most likely keyhole voids.

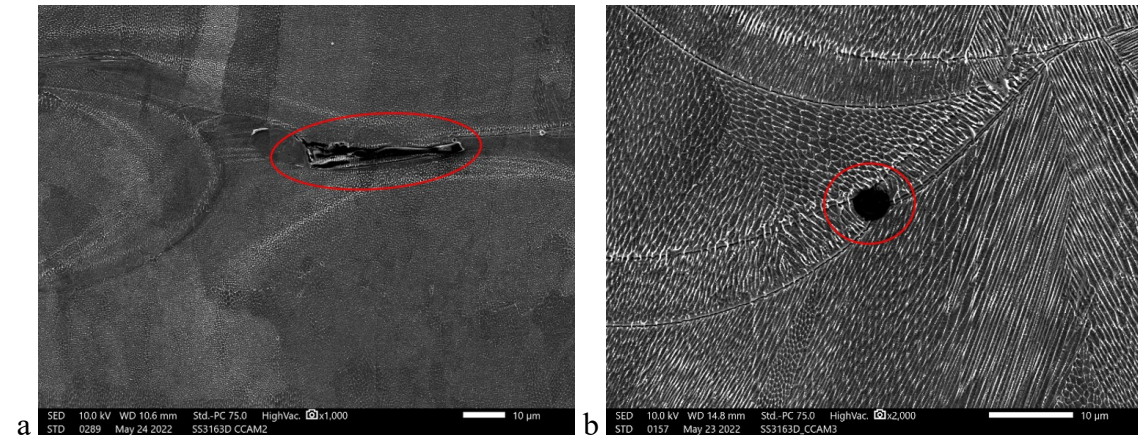


Figure 2.11: SEM images of highlighted defects from a) the group 2 sample viewed along the z direction at a magnification of 1,000x and b) the group 3 sample viewed along the x direction at a magnification of 2,000x.

The elongated shape and irregular edges of the group 2 defect highlighted in Fig. 2.11a are characteristic of lack of fusion voids, caused by insufficient melting of the powder material. This leaves a cavity in the material with a rough surface finish and non-uniform shape. In contrast, the defect from the group 3 sample shown in Fig. 2.11b is very round and uniform in shape with smooth edges, suggesting that this is a keyhole void.

The likelihood of finding lack of fusion or keyhole voids has been shown by Liu et al. (2020) [25], Agrawal et al. (2020) [31], and others to be associated with the VED used to process the material. It was shown that for higher VED, keyhole voids are more likely to be created, and when the VED is too low, lack of fusion voids are likely to form. The higher VED used to process the group 2 samples compared to the group 3 samples does not match this expected trend with lack of fusion voids creation. The laser power used for group 2 was lower than group 3, which is directly related to a decrease in the

input energy and localized material melting. This suggests that laser power could have a strong influence on the development of lack of fusion voids in SLM parts in addition to, and possibly more so than, the VED.

The area percent defect content was recorded for each image of each sample and the results are displayed in the histograms of Fig. 2.12 below along with the Weibull distributions fitted to the data. The Weibull distribution was selected for the curve of best fit to represent the data presented in this study because the Weibull distribution accurately predicts a probability of zero for values less than zero and the Weibull distribution accurately represented the skewed trend of most of the data as evident by a high R-square value above 0.9 for most data sets.

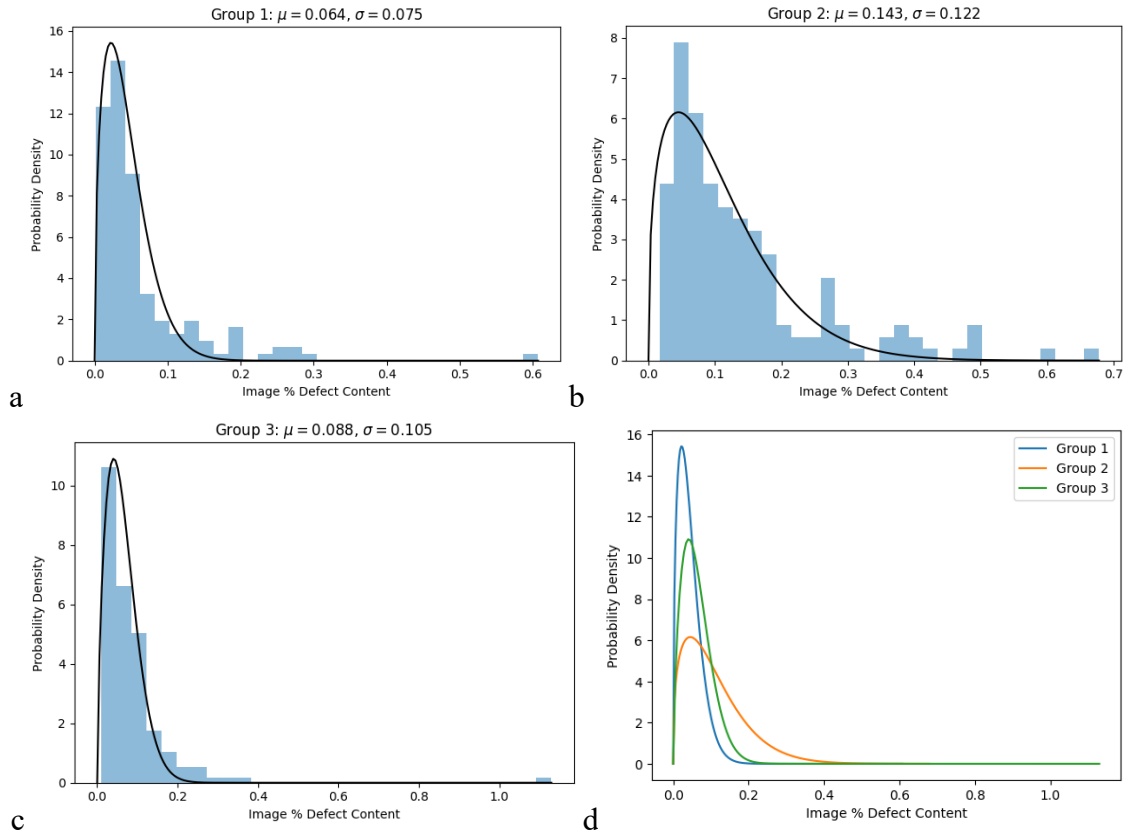


Figure 2.12: Percent void content data measured by a custom Python script utilizing traditional image processing techniques on optical sample images. Histograms of the percent defect content measurements are plotted for sample group 1, 2 and 3 in a, b and c respectively. The mean and standard deviation of each sample group data set are shown. Fitted Weibull distributions of each data set are also shown and are plotted together in d for comparison.

Overall, the defect content of all the sample groups measured very low, with the density of most samples predicted to be greater than 99.8%, which is beneficial for the mechanical properties of the parts according to experimental results from Liu et al. (2020) [25] and simulation results from Ahmadi et al. (2016) [54]. Sample group 1 measured the lowest standard deviation in percent defect content and sample group 2 the highest, nearly twice that of group 1. Sample group 1 also measured the lowest average percent defect content and sample group 2 the highest, slightly more than double that of group 1. The density measurements obtained here are very similar to the results reported by Agrawal et al. (2020) [31] for 316L SS parts manufactured with similar fabrication

processing parameters above 70 J/mm³ VED, in which the density measurement is suggested to be relatively insensitive to changes in VED. As expected, the density measurements obtained here are higher than the findings of Suryawanshi et al. (2017) [27] where part densities of about 98% were recorded, due to different fabrication processing parameters for the same material resulting in a lower VED of only 20 J/mm³.

The quantitative results of the sample defect measurements are summarized in Table 2.3 below and agree with the qualitative analysis results. The group 2 sample measured the highest defect content and the group 1 sample the lowest. The group 2 sample also measured the highest average defect area, while the group 1 and 3 samples measured similar average defect areas, nearly half that of the group 2 sample. The standard deviation in both the image defect content and defect area trends with the average values for each sample so that the group 2 sample measured the highest standard deviation and the group 1 sample the lowest. The group 3 sample measured the highest number of defects per unit area, slightly higher than the group 2 sample. The group 3 sample has a smaller image defect content than the group 2 sample despite measuring a higher defect count because the average defect count is only slightly higher, but the average defect area of the group 2 sample is nearly double that of the group 3 sample. Both the mode and median of the defect area measurements are very similar between each test group and are much lower than the average values. The mode and median values being much lower than the averages suggests that there is a much larger amount of very small defects compared to large defects in all of the samples.

Table 2.3: Tabulated summary of some of the defect metrics for each sample group. The image defect content is the percentage of pixels representing a defect compared to the total number of image pixels and is also shown plotted in the histograms of Fig. 2.10 above. The defect area measurement is the area in square microns of each defect detected by the custom Python script. The defect count is an area-normalized measure of the average number of individual defects per square mm for each sample group.

Group	Archimedes Volumetric Porosity Content (%)	Image Defect Content (% area)				Defect Area (μm ²)				Defect Count (#/mm ²)
		Average	Mode	Median	Standard Deviation	Average	Mode	Median	Standard Deviation	Average
1	1.34	0.064	0.016	0.039	0.075	7.711	0.292	1.753	46.688	82.6
2	1.13	0.143	0.089	0.105	0.122	12.350	0.292	2.045	64.601	115.7
3	0.71	0.088	0.038	0.061	0.105	7.390	0.292	1.753	51.251	118.5

The results of the Archimedes' density measurements are also shown in Table 2.3, displayed as the percent volume content of voids within the sample from each group. The Archimedes' void content density measurements were higher than the void content estimates from the image analysis method, with the Archimedes results more closely matching the findings of Suryawanshi et al. (2017) [27] who tested parts manufactured with much lower VED. The trends in Archimedes and image analysis results with defect content measurements between sample groups also did not match, which was not expected. The Archimedes results suggest that the expected part density decreases with increased VED, which contradicts the defect content results from the image analysis and the findings of Agrawal et al. (2020) [31].

Given that over 50% of the observed defects are less than 7 px, equal to 2.045 μm², in total size, some accuracy is lost due to the magnification and image resolution

chosen. However, a single pixel represents a length of only $0.54\text{ }\mu\text{m}$ and an area of about $0.292\text{ }\mu\text{m}^2$, which is less than 0.0001% of the total surface area captured within a single image. If the void instance segmentation accuracy is within ± 4 px for each detected void, which is likely an over-estimate of the amount of error, the final defect content measurement is only altered by $\pm 0.05\%$ points. This is assuming that all the defects within an image are 7 px in area (± 4 px) and the total number of defects is increased to match the measured average defect content.

To a similar effect, the accuracy of the segmentation masks for larger defects is reduced near the boundary of the defect due to the image resolution. This error is expected to be proportional to the perimeter of the defect but is still not a considerable source of error in these measurements. As the size of a single defect increases, the perimeter increases linearly, and the measured surface area increases quadratically. The percent error in the area measurement due to resolution inaccuracies near the defect edges increases at a rapidly diminishing rate with defect size, and the error for very small voids has already been shown to be negligible. Therefore, the expected error in the defect area measurements due to the image resolution has only a small effect on the results and is considered negligible.

The defect detection tool developed here is expected to provide defect content, size and count information for most digital optical images resembling the raw optical images, such as those shown in Fig. 2.10, captured here. For the best results, the defects should have a high contrast from the polished surface of the sample, and the number of visible features other than defects should be minimized. Any scratches, shadows, contaminants and other features on the sample surface will likely appear as dark features and the tool will likely erroneously interpret these features as defects. The magnification or dimensions of images analyzed by the tool will not affect the segmentation ability of the tool, but as discussed above, can affect the measurement resolution, and therefore affect the expected accuracy of the measurements.

The relatively high part densities measured for each sample group suggests that the fabrication processing parameters used here are adequate for creating 316L SS SLM parts. Both the qualitative and quantitative analyses showed predominantly keyhole voids in the samples, with an increased amount of lack of fusion voids observed in the group 2 sample due to the lower laser power during processing. The defect area measurement error due to the image resolution was investigated and determined to be insignificant for the results obtained here. Part densities of additional samples need to be measured using both the Archimedes' and image analysis methods to test the variance of the results and accuracy of both methods, ideally with a larger test window of fabrication processing parameters to aid in identifying trends between defect content and fabrication processing parameters.

2.4.3 Cell Characterization Results

Figure 2.13 below shows example bounding box and segmentation mask prediction outputs for two images that were not included in the training or validation data sets. A uniquely colored segmentation mask is created for each detected cell instance. A classification confidence score ranging from 0 to 1 is also assigned by the model to each instance to describe the certainty that the detected geometry belongs to the cell class, with 0 being least confident and 1 being most confident. Only detected cell instances with a

classification confidence value above 0.97 are accepted by the model, cell instances with a confidence score below 0.97 are automatically removed from the output and ignored. The classification confidence values for the cell objects in this study are expected to be high because there is only a single cell class being examined.

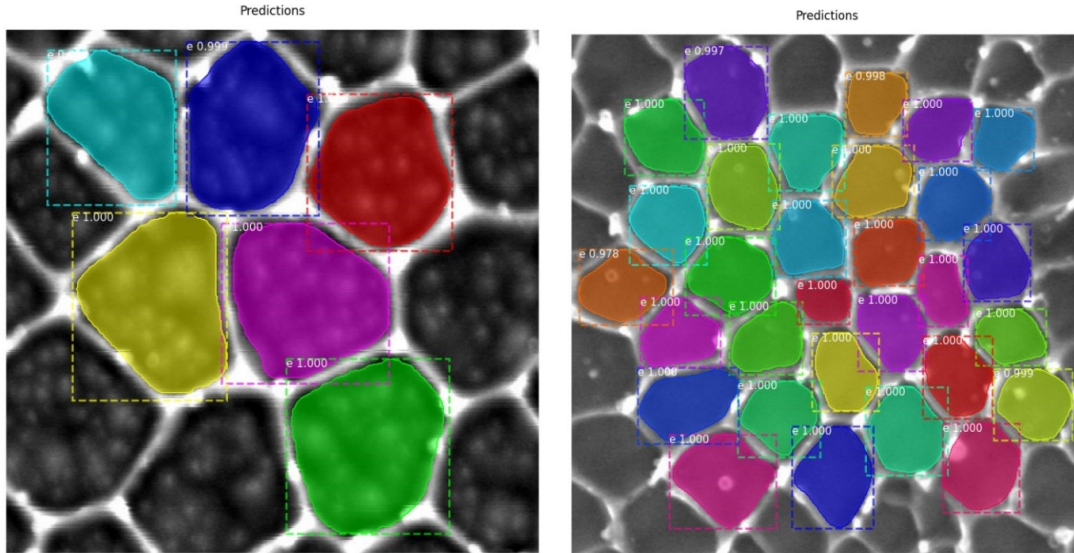


Figure 2.13: Two example prediction outputs from the trained Mask R-CNN model showing the ability of the trained model to identify cell instances and produce segmentation masks with a relatively high degree of accuracy. Each segmentation mask is randomly colored, and a decimal number is given in the upper left corner of each instance bounding box to represent the classification confidence score from 0 to 1. Both images are 512 by 512 px sections of different 10,000X magnification SEM images that were not included in the training or validations data sets.

Qualitative inspection reveals that the cell segmentation masks accurately represent the cell objects, and the results are equivalent to the accuracy expected by manually produced segmentations. Most of the visible errors are only small underestimations in the cell area where the segmentation masks do not extend all the way to the lighter colored cell boundary material. The relatively high accuracy of the segmentation masks suggests that the differences in cell sizes, image brightness, image contrast, and other microstructural features do not interfere with the ability of the Mask R-CNN model to correctly identify and segment the cells in the images. It is also observed that the cells near the edges of the image which are not fully in view are correctly ignored.

The images shown in Fig. 2.14 below provide a direct comparison between the model predicted segmentation masks and the manually annotated ground truth segmentation masks for four SEM images from the validation data set.

Ground Truth and Predictions
GT=green, Pred=red, captions: confidence score/IOU

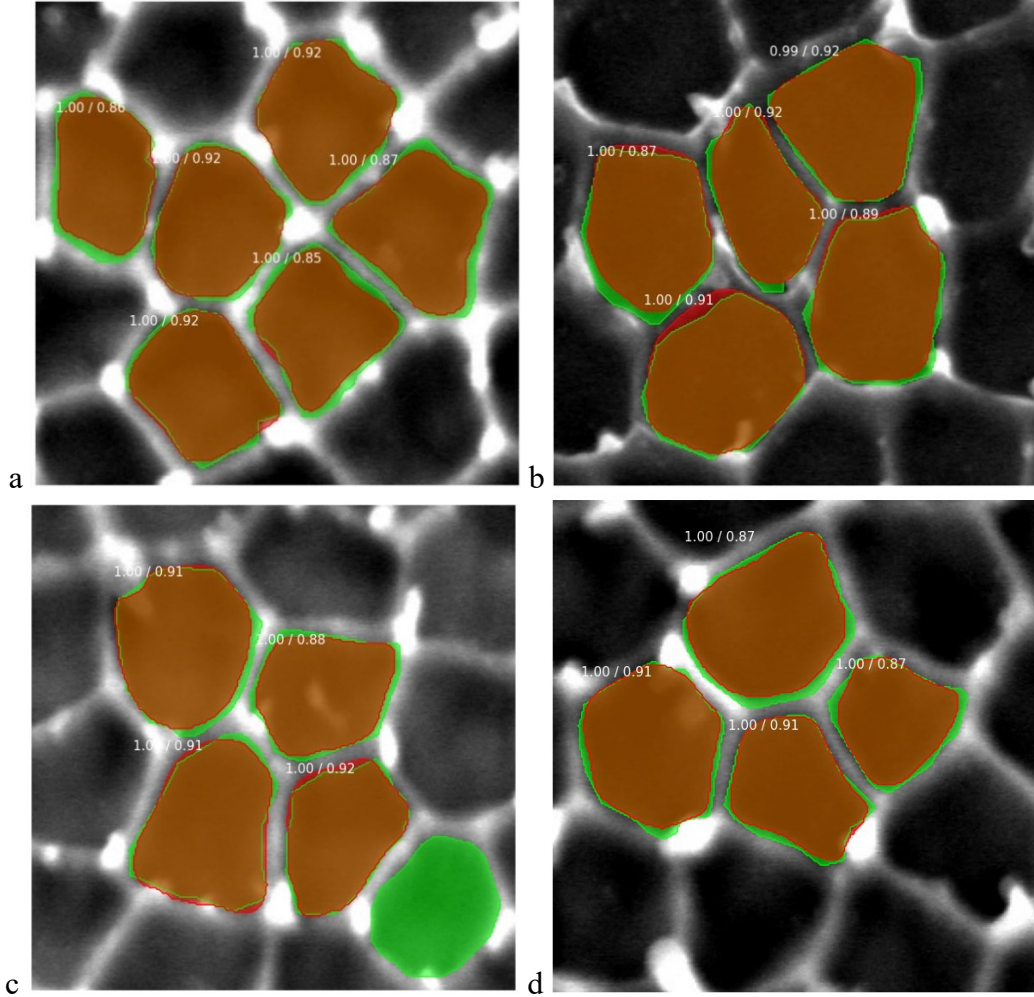


Figure 2.14: Comparison of the red model predicted segmentation masks with the green annotated ground truth masks for four different 256 x 256 px images from the validation data set. The confidence and IOU scores are also shown for each detected cell.

Overall, the red segmentation masks predicted by the model closely match the green ground truth masks. Some error is observed near the edges of the cell object where the model often predicts a slightly smaller segmentation mask than the ground truth mask. The IOU scores displayed with each cell instance, ranging between 0.87 and 0.92, also suggest quantifiably that the model predicted masks are similar to the ground truth masks. The distribution of IOU scores for each detected cell instance within the validation data set is shown in Fig. 2.15 below. In some cases, false negatives are observed in which the model fails to predict a cell instance included in the ground truth annotations. This is represented in Fig. 2.14 above by the green segmentation mask with no accompanying red model predicted segmentation mask to represent the same cell object. The false negatives predicted by the model do not affect the measurements

because they do not add a datum point to the data set and are therefore not relevant to this application.

All cell instances predicted by the model but not present in the ground truth, referred to as false positives, were removed from the data set and ignored when presenting the IOU scores. A total of three false positives were detected in the validation data set. Two of the false positive cell instances were fully visible and could have been included in the ground truth annotations, so these false positives do not represent an error from the model. One edge of the last false positive instance was not fully visible within the image and therefore the instance should not have been selected by the model. This false positive represents an error from the model, but only represents an error rate in selection of about 1% and the error introduced into characterization metrics is even lower. Due to the three false positives introducing little or no expected error into the model prediction results, these outliers, which would measure IOU scores of 0, were removed from the data.

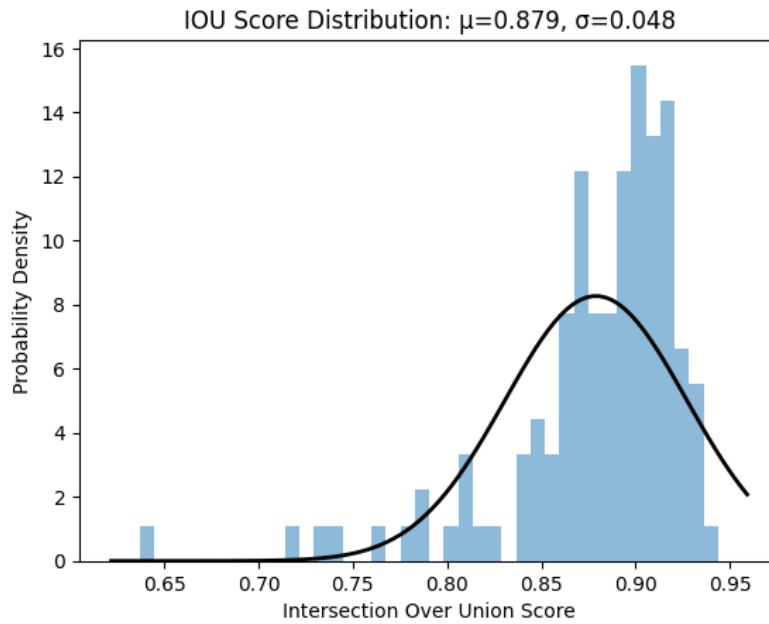


Figure 2.15: Intersection over union (IOU) score distribution for all validation data set cell instances detected by the model. A best-fit Weibull distribution is plotted as a black line.

The model measured a high average segmentation mask IOU score of 0.879, high mode of 0.90 and low standard deviation of 0.048 for the cell instances within the validation data set. About 90% of the detected cell instances measured an IOU score above 80%, which indicates a high segmentation accuracy for a large amount of the data. These IOU metrics suggest that the model is sufficiently trained to provide accurate cell instance segmentation data from SEM images for computing cell characteristics. To further support the reliability of the measurements produced by the model outputs, the distribution of cell area measurements calculated from the ground truth and model prediction segmentations are compared in Fig. 2.16 below along with the best fit normal distributions for both data sets. The normal distribution is chosen to represent these data sets instead of the Weibull distribution used for other data sets in this study because the best fit Weibull distribution did not accurately represent the data, with an R-square value

below 0.3. The fitted normal distribution better represented these data sets with a higher R-square value near 0.6.

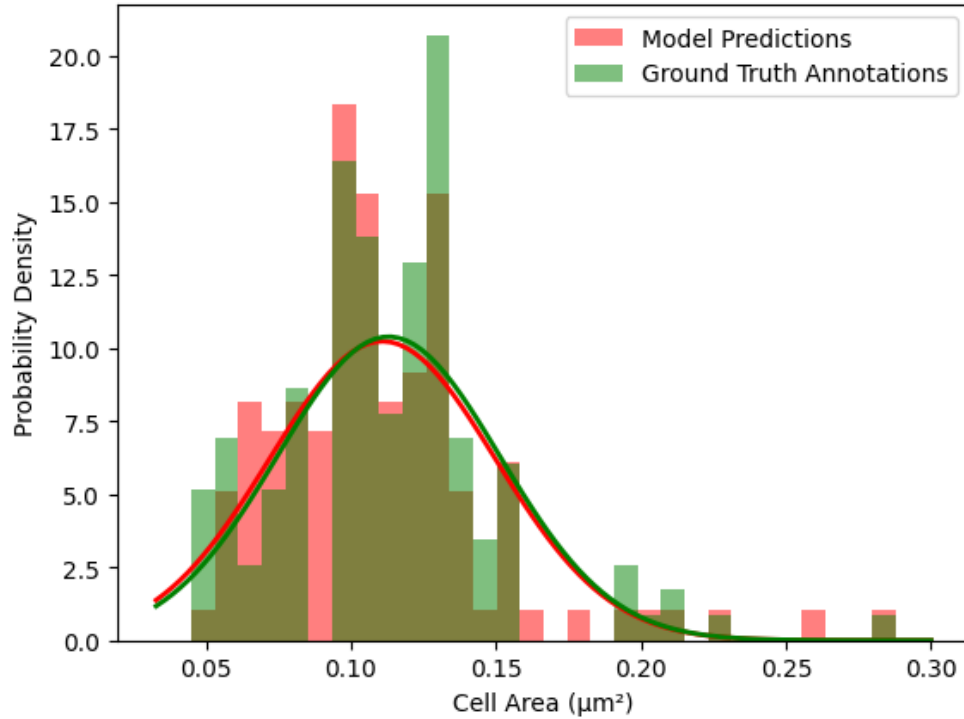


Figure 2.16: Comparison of measured cell area distributions from the validation data set calculated by the ground truth, green, and the model prediction, red, segmentation masks. Fitted normal distribution curves computed from the mean and standard deviation values for both data sets are also shown. The normal distribution was chosen rather than the Weibull distribution used for other results presented here because parameters for a well fit Weibull distribution were not found for these data sets.

The relatively small differences between the ground truth and model prediction segmentation masks analyzed above have a very small effect on the resulting distribution of cell area measurements. The distributions of cell area measured from the ground truth masks and prediction masks are very similar to each other, and the comparison of the fitted normal curves of both data sets reveal very little difference in both the average and standard deviation. The data in Table 2.3 below shows a comparison in the measured mean and standard deviation values from the ground truth and model prediction sources. The similarity of the cell area measurements suggests that the outputs produced by the model are equal in quality to that of manually processed images. It also suggests that the differences in the model outputs from the manual annotations are minimal and do not affect the characterization measurement results of importance here.

Table 2.4: Summary of the mean and standard deviation values for the cell area measurements calculated from the ground truth and model prediction segmentation masks.

Measured Cell Area (μm^2)		
Source	Average	Standard Deviation
Ground Truth Annotations	0.1129	0.0384
Model Predictions	0.1108	0.0390

Having provided evidence for the high accuracy and reliability of the model segmentation mask predictions used to calculate the cell characteristics, the results of the cell area measurements provided by the model predictions are shown below in the histograms of Fig. 2.17. Each data point represents the cross-sectional area in μm^2 of a single cell for a given sample group.

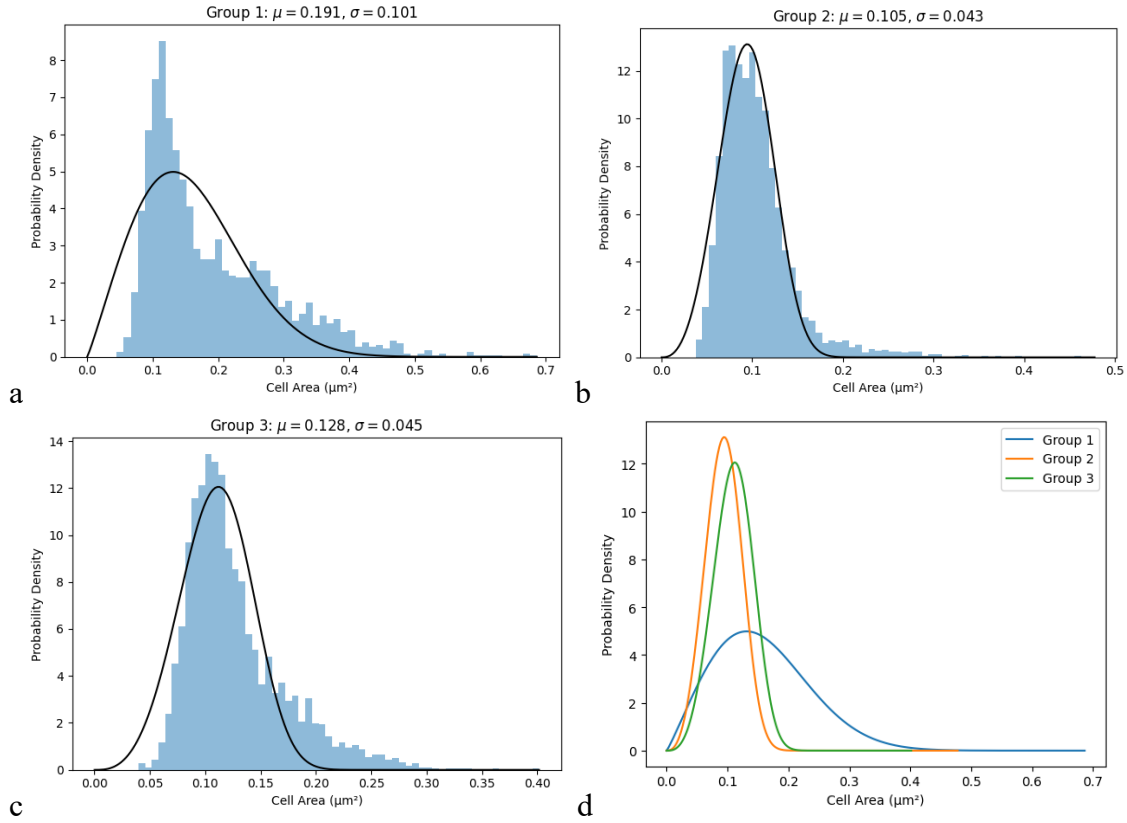


Figure 2.17: Cell area data measured by the Mask R-CNN model from the SEM images are plotted for groups 1, 2 and 3 in a, b, and c respectively. The sample population average and standard deviation measurements are shown for each sample group. Fitted Weibull distributions are also plotted for each data set and shown together in d for comparison.

The image data set for each group is composed of about 200 512 x 512 px images subdivided from the SEM images captured earlier. None of the images used here and beyond for cell area or PDAS measurements were used within either the training or validation data sets. The average cell area values and standard deviation of each sample group are also shown in Table 2.5 below.

Table 2.5: Summary of the cell area measurements for the three sample groups, showing the average and standard deviation measurement statistics.

Cell Area (μm^2)		
Group	Average	Standard Deviation
1	0.191	0.101
2	0.105	0.043
3	0.128	0.045

Sample group 1 measured the highest average cell area, 1.5 times larger than the next closest group, as well as the highest standard deviation by 2 times that of the other groups. Sample groups 2 and 3 share similar cell area distributions, with the standard deviation of sample groups 2 and 3 being nearly identical and the average cell area of group 3 measuring only slightly higher than that of group 2.

The PDAS measurements were obtained by post processing the Mask R-CNN segmentation mask outputs as described in section 2.3.3, and the distributions of the resulting data are shown in Fig. 2.18 below for each test group. The PDAS results are very similar to the cell area results for each sample group as expected because these two measurements are directly related to one another.

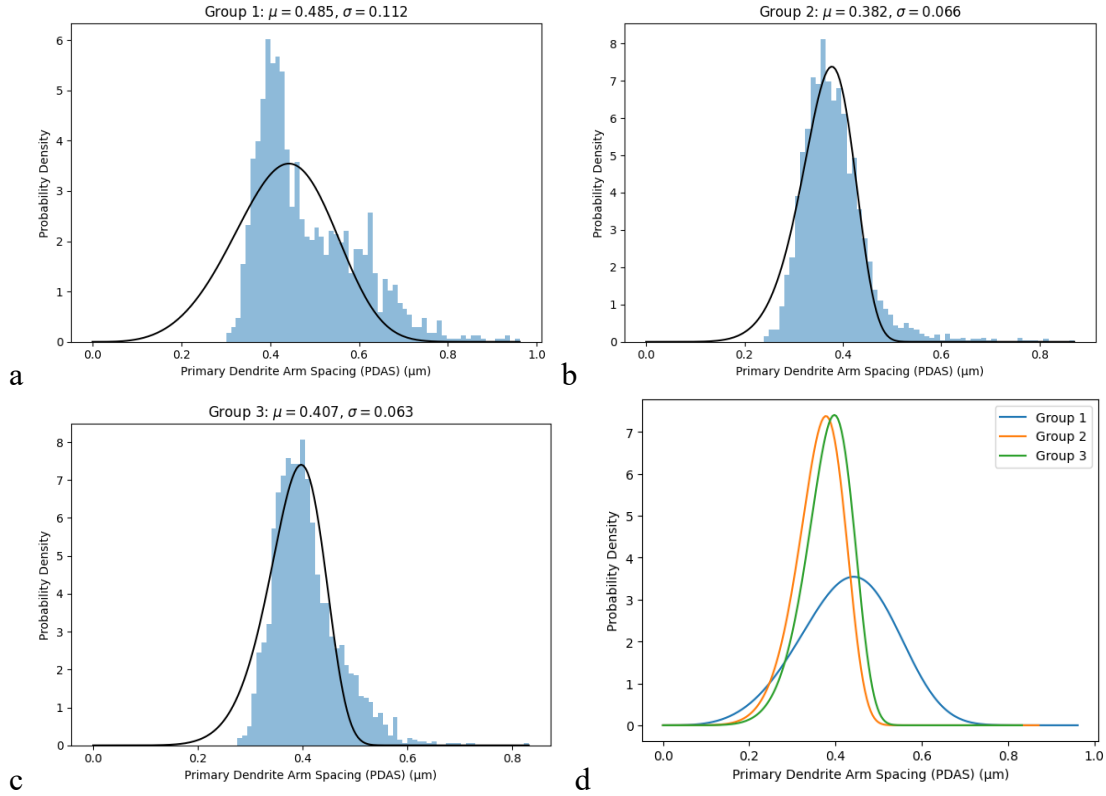


Figure 2.18: Primary dendrite arm spacing data distributions measured by the Mask R-CNN model segmentation predictions from the SEM images are plotted for groups 1, 2 and 3 in a, b, and c respectively. The average and standard deviation measurements are shown for each sample group. Best fit Weibull distributions for each data set are also shown and plotted together in d for comparison.

Just as for the cell area results, sample group 1 measured the highest average value and standard deviation of PDAS. The mean and standard deviation of sample groups 2 and 3 were very similar, with sample group 3 measuring a slightly higher average value, as was the case for the cell area measurements. A summary of the measured average and standard deviation values of the PDAS results for each sample group are shown in Table 2.5 below.

Table 2.6: Summary of the mean and standard deviation values for the primary dendrite arm spacing (PDAS) measurements of each group.

Primary Dendrite Arm Spacing (μm)		
Group	Average	Standard Deviation
1	0.485	0.112
2	0.382	0.066
3	0.407	0.063

The PDAS results obtained here closely match the PDAS measurements from Agrawal et al. (2020) [31] in which a larger number of samples were tested with various fabrication processing parameters. The findings of both studies show a direct trend in PDAS with VED. The PDAS measured here follow the linear relation with VED proposed by Agrawal et al. (2020) [31], but the measurement of the group 2 PDAS is lower than expected.

The higher mean and variance in the group 1 cell size is most likely a result of the increased laser power and VED used to process this sample group. Sample group 1 measured the highest cell size and was printed with the highest laser power and VED, measuring 125 J/mm^3 , while groups 2 and 3 were printed with VEDs of about 90 and 73 J/mm^3 respectively. The group 2 samples were manufactured with the lowest laser power of 150 W, but only the second lowest VED, and measured the lowest average cell size. This suggests that the laser power parameter could be a more important metric for estimating the cell size and therefor has a larger effect on the thermodynamic development of the material due to the stronger correlation of cell size with laser power than VED as concluded by Agrawal et al. (2020) [31]. Other fabrication processing parameters, such as hatch spacing and scanning speed, have been shown by Stephen (2021) [39] to affect the expected cell size measurements, but to a lesser degree than the laser power or VED. Additional cell size measurement data from more samples manufactured with a range of fabrication processing parameters will be required to accurately correlate the fabrication processing parameters with expected cell size.

The exact mechanisms that create the cellular microstructure observed in the SLM 316L SS samples are not fully understood, but it has been shown that the selection of VED affects the final geometry of the cell structure. According to Prashanth and Eckert (2017) [14], both thermodynamics and kinetics play a key role in the cell structure formation and altering the VED directly effects the thermal conditions during processing.

The measured cell size is thought to increase with higher VED due to the larger volume of melted material and extended liquidous period when melted. Both the Bernard Marangoni driven instability (BMI) and particle accumulated structure formation (PAS) mechanisms used to describe and predict cellular microstructure formation suggest that

the cell structure is formed by segregation and mass transport of alloying elements during processing [14]. A larger volume of material molten for a longer period can facilitate the preferential mass transport suggested by the BMI and PAS mechanisms throughout a larger volume for a longer amount of time, creating larger areas of coalesced alloying elements. This results in larger cell sizes observed in the final structure. This agrees with the experimental observations made by Katayama and Matsunawa (1984) [15] who suggested that the cooling and solidification rates of the SLM process was the reason for lack of solute diffusion and redistribution, therefore leading to smaller microstructural cell features. The authors presented an empirical formula to approximate the PDAS based on the measured material cooling rate.

The Mask R-CNN model and cell size measurement methods used here were shown to be accurate and reliable for the samples tested, but some potential sources of error still exist when comparing the cell size results between groups. Primarily, the SEM images captured from each sample group are assumed to be representative of the entire cell structure of each part within the test group, but the captured images are only a very small fraction of the total volume of a single part.

Given SEM images for analysis similar to those shown in Fig. 2.6, the cell characterization tool is expected to provide accurate cell area and PDAS measurements for material samples according to the accuracy estimations presented above. Imaged cell structures analyzed by the tool developed here should feature dark cells and lightly colored cell boundaries, and images should be captured from areas of the cell structure where the cells appear round. It is recommended that imaged to be analyzed by the tool have dimensions no greater than 512 x 512 px and that the images be captured near 10,000x magnification so that the cell diameter is roughly near 0.5 μm . These image settings will ensure that the cells in the imaged cell structure closely match the imaged cells of the training dataset. This similarity between cells in new images and the training data set images will give the Mask R-CNN model the best chance to accurately predict new cell segmentations. Images of cell structures which do not resemble the images shown in Chapter 2 or that are of a much larger dimension than specified will likely not produce the high segmentation accuracies measured here.

Images were captured viewing along the z direction of the part to align with the preferential growth direction, but it is unknown if the measured cell size is related to the growth direction or even if this trend is constant for different fabrication processing parameters. Also, results from Saboori et al. (2019) [28] have shown that the microstructure characteristics of AM materials such as PDAS are dependent upon the height from the substrate due to variation in the cooling rate and thermal gradient. This implies that for a single sample, the cell size measurements are expected to be different depending on the cross section chosen for imaging. Although it was attempted to image all the samples in this study within the bulk of the material away from the part edges and at a consistent cross section depth, the depth location accuracy cannot be guaranteed.

2.4.4 Material Characterization Results Summary

Both the defect and cell imaging characterization methods presented and used here offer a relatively simple and effective strategy for material microstructure characterization. The two-dimensional imaging provides adequate resolution for measurement accuracy and sensitivity, and the data can also be used for qualitative

analysis. The major disadvantage of the imaging characterization methods presented is that the results are reliant on the collected images from a relatively small proportion of the sample volume being representative of the bulk material. For many randomly sampled images, this is a decent assumption, but microstructure characteristics have been shown in previous studies to vary with distance from the substrate and even distance from part edges, which could skew results depending on the cross section height the images are sampled from [28]. Given the complexity and time needed to prepare a unique sample surface for imaging, the simplicity of the image analysis tool developed here diminishes if many cross sections are examined. The results of the defect content measurements also did not match the Archimedes density measurements as closely as expected. However, the trends in the results of the Archimedes measurements were not in agreement with the results of other studies investigating similar samples of the same material.

The group 1 samples measured the lowest average percent defect content and total number of defects as well as the highest yield and ultimate tensile strength, similar to the findings of other studies relating yield and ultimate tensile strength with defect content [25], [54]. In contrast with these studies, the group 3 samples which measured the lowest yield and ultimate tensile strength did not measure the highest percent defect content. The group 2 samples instead measured the highest percent defect content and highest average defect area but measured a slightly higher experimental ultimate tensile strength than the group 3 samples. The group 3 samples did, however, measure a higher number of voids than the group 2 samples, indicating that the number of defects might have a larger effect than the size of defects on the material tensile yield strength.

The group 1 samples also measured the largest average cell size, likely due to the high laser power and VED during manufacturing. The relation between the high tensile yield strength and high average cell size measured in the group 1 samples relative to the other groups is in agreement with the MD simulation results obtained by Kurian and Mirzaeifar (2020) [48], but in contrast with the experimental findings of Agrawal et al. (2020) [31] who suggested that the yield strength increases with decreased cell size according to the Hall-Petch relationship. However, the results here do not show a clear and consistent trend in yield strength with cell size, likely because the yield strength is dependent upon many factors other than the cell size alone. Again, more data is required from additional samples to provide strong evidence for trends linking the material performance to the part structure and fabrication processing parameters.

3 Melt Pool Structure Computational Modeling

3.1 Introduction

The simulation work completed by Ahmadi et al. (2016) [54] provided a great method for investigating the mechanical response relationship between the melt pools, grains and even voids of a typical SLM structure. However, the semicircle melt-pool geometry assumption does not accurately represent observed geometries and limits the insight gained from comparing different geometries created by various fabrication processing parameters.

In this work, a custom melt pool structure generation tool is developed to create realistic melt pool structures with melt-pool geometries that can easily be controlled with a few simple user inputs and varied along any dimension of the structure. It is also required that the melt pool structure generation tool creates completely enclosed melt-pool geometries so that the results can be used reliably in FEA models.

The tool proposed here is intended to serve as a part of the virtual testing framework for AM parts and is presented here in a simple form with uniform material definitions for each melt pool. The melt pool structure-based analysis proposed here is intended to enable other simulations methods, utilizing models such as crystal plasticity, molecular dynamics, etc., to use more complex and physically representative melt-pool geometries to represent material interactions at larger length scales.

3.2 Custom Melt Pool Structure Model

The melt-pool geometry model used here was created using Abaqus and custom Python scripts. The custom model is intended to be the foundation for a mesoscale virtual testing framework for SLM AM structures. The melt pool is used as the base geometric building block with uniform material definition throughout a single melt pool. Details of the melt pool structure are 2-dimensional in the Y-Z plane of a single scan direction material as described in section 2.1. Each melt pool is represented as a completely enclosed geometry comprised of intersecting parabolas as shown below in Fig. 3.1. Using a few simple inputs, a wide variety of realistic 2-dimensional single laser scan direction melt-pool geometries can be created with uniform or varying properties and material definitions.

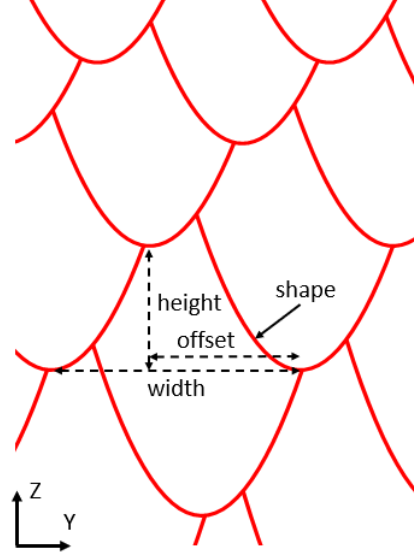


Figure 3.1: Section of example melt pool structure built by plotting unique intersecting parabolas.

The parabolic geometry was selected to represent SLM melt pools as an improvement from the semi-circle geometry previously used by Andani et al [55], Ahmadi et al [54] and other studies, and assumes that the laser beam used for SLM processing has a parabolic energy profile, which is very similar to the gaussian energy distribution typically assumed.

The 2-dimensional melt pool structure is based on four user inputs which describe the desired melt pool dimensions. The four inputs are referred to as the width, height, shape and offset parameters. The inputs of width and height for each melt pool define the respective x and y spacing between neighboring parabola vertices and are analogous to the hatch spacing and layer height inputs commonly controlled in SLM processing. The shape parameter is used to define the profile of each melt pool and represents the effect of multiple fabrication processing parameters in combination which determine the curvature of the melt pool. For example, processing a part with high laser power and low scanning speed is more likely to produce a deep and narrow melt pool, which is represented by a high shape parameter value. In contrast, using a reduced laser power and scanning speed is likely to produce a shallow and wider melt pool, represented by a low shape parameter value [64]. The width, height and shape modeling parameters shown in Fig. 3.1 are used to describe each parabola according to the parabola vertex form shown in Eq. 3.1.

$$y = a * (x - h)^2 + k \quad (3.1)$$

The shape parameter is given as a , and the width and height parameters are associated with the (h, k) location of the vertex. The offset parameter is used to define the x-direction distance between adjacent layers. The parameters chosen for each melt pool are used to plot parabolas sequentially starting with the uppermost layer and proceeding right to left then top to bottom. This method ensures that there are no gaps or overlapping of MPBs and mimics the geometry created by melt pool remelting from adjacent and upper layers observed in SLM processed structures.

Based on the chosen user input parameters, many different melt-pool geometries can be constructed to accurately match real observed melt-pool geometries. A range of

geometry values are selected and used to create the melt pools shown below in Fig. 3.2 to show some of the potential melt-pool geometries.

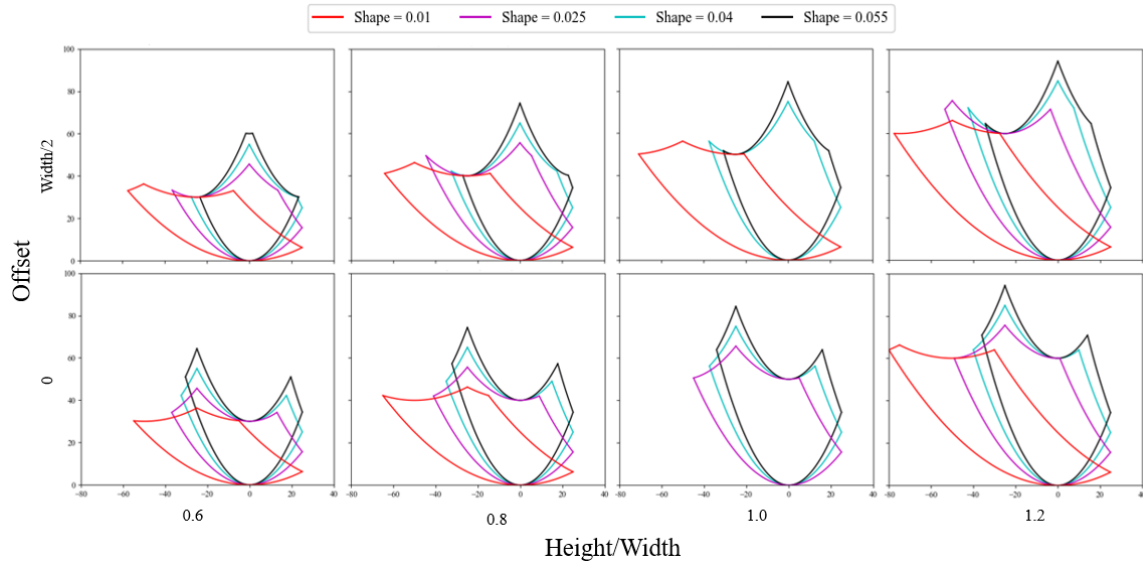


Figure 3.2: Example melt-pool geometries created with custom melt pool generation tool to show some of the possible geometries and the effect of the user input parameters on the resulting geometry.

The four user input parameters that describe the melt-pool geometry can also be varied spatially within the melt pool structure to create graded melt pool structures simply and effectively. The width, height, shape and offset of each melt pool can be defined uniquely according to user defined functions or specified for each location. Realistic melt-pool geometries which would be difficult to create manually with repeating patterns and perfectly enclosed geometry are now simple to construct without significantly sacrificing customization or accuracy. An example of a graded melt pool structure in which the height and shape parameters are varied periodically with the layer height is shown in Fig. 3.3 as it would appear in Abaqus and the corresponding trend in input geometry parameters with layer height is shown.

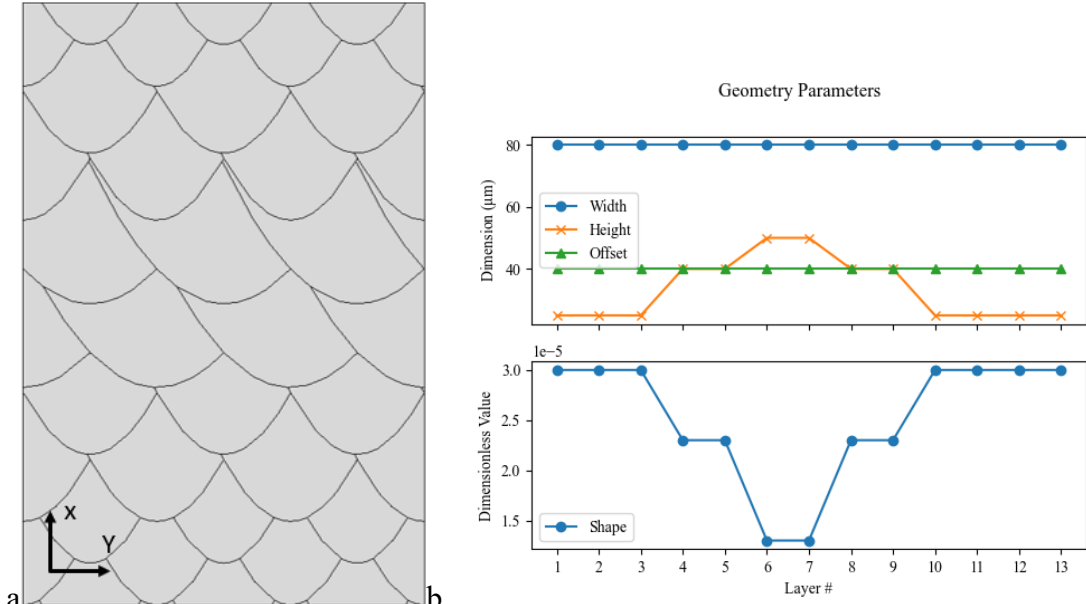


Figure 3.3: Example melt pool output showing a) the melt pool structure as seen in Abaqus for stress analysis, and b) the plot of the variation of user defined geometry parameters which define the morphology and distribution of the melt pools.

In this example, the parameters for two consecutive layers are kept constant then changed for the next consecutive layers, with the parameters mirrored halfway along the height to create a periodically repeating structure. Each grouping of constant geometry parameters represents layers produced with the same fabrication processing parameters. Within the Abaqus simulation space, the height dimension of the part is referred herein as the y direction, and the width dimension is referred to as the x direction as shown in Fig. 3.3a.

3.3 Modeling Methods

For the example structure shown above in Fig. 3.3, the layers produced with identical fabrication processing parameters are assigned identical material properties. The material property definitions for each layer grouping can be seen in Fig. 3.4 below, where each color indicates a unique material definition corresponding to the similarly colored engineering stress vs engineering strain plot in Fig. 3.4b.

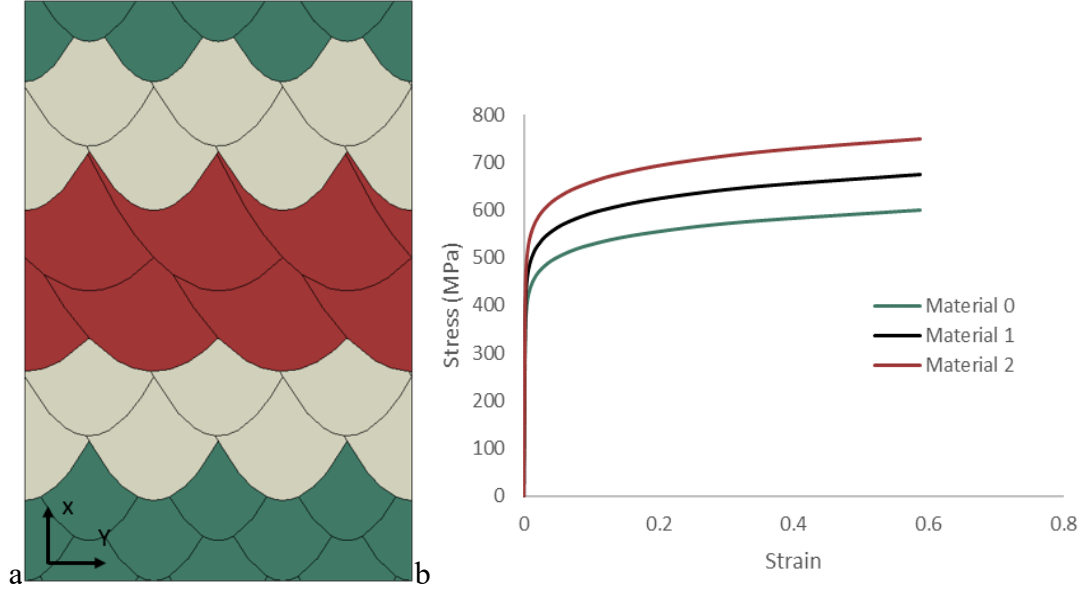


Figure 3.4: The same melt pool structure shown in Figure 3.3 is color coded to show each unique material definition a) in the melt pool structure and b) plotted according to the Ramberg-Osgood material response defined for each material. The engineering stress and engineering strain is plotted.

The specific properties assigned to each material follow the Ramberg-Osgood material model presented in Eq. 3.2 and are input into Abaqus using the elastic plastic material model as true stress and true strain. The elastic modulus and Poisson's ratio define the elastic response of the material, and the plastic response is defined by entering the tabulated true plastic strain and true stress from the Ramberg-Osgood equation.

$$\varepsilon = \frac{\sigma}{E} + \frac{\alpha * \sigma}{E} \left(\frac{|\sigma|}{\sigma_0} \right)^{n-1} \quad (3.2)$$

Here, σ represents the independent variable for true stress, ε is the dependent variable for true strain, E is the elastic modulus, n is the hardening exponent, σ_0 is the yield stress and α is the yield offset which is defined according to Eq. 3.3 such that yield is defined by the 0.2% offset method.

$$\alpha = \frac{0.002 * E}{\sigma_0} \quad (3.3)$$

The 0.2% offset method is used to estimate the yield point of a material given the stress vs strain curve of the material. To estimate the yield point of a material using the 0.2% offset method, the linear elastic modulus of the material, the slope of the elastic region, is measured and translated 0.002 mm/mm along the positive x axis. The point at which the offset linear elastic modulus intersects the stress vs strain curve is estimated as the yield point of the material. The 0.2% offset method is a repeatable way to estimate the yield point of a material even for materials with different yielding behaviors.

The material properties chosen for the example shown in Fig. 3.4 are shown in Table 3.1 and represent example material strengths which might be produced by varying the SLM fabrication processing parameters. The exact values chosen are not based on

previous data, but instead were chosen to analyze stiffness and yield strength mismatches between adjacent layers.

Table 3.1: User selected Ramberg-Osgood material properties defining the three materials.

Material	Elastic Modulus (GPa)	Poisson's Ratio	Yield Stress (Mpa)	Hardening Exponent	Yield Offset
0	160	0.33	400	14	0.8
1	180	0.33	450	14	0.8
2	200	0.33	500	14	0.8

With the geometric structure and materials defined, a compatible mesh is created for the melt pool structure geometry so that the elements of neighboring melt pools share the same nodes at MPBs. The nodes at apposing domain edges are also aligned with each other to be compatible. The CPS4R, a 4-node bilinear plane stress quadrilateral, reduced integration, element type is chosen for the 2-dimensional analyses in the following sections.

Periodic boundary conditions (PBCs) are applied to the representative volume element (RVE) geometry domain Ω_{RVE} to simulate the bulk material response. The PBC creates a periodic relationship between the compatible nodes of the left and right edges as well as between the compatible nodes of the top and bottom edges. This boundary condition choice is justified by van der Sluis et al. (2000) [57], Terada et al. (2000) [65], and others who showed that PBCs give a more accurate estimation of the effective moduli than other boundary conditions such as uniform displacement or uniform traction when applied to a RVE. The example melt pool structure from above is shown below in Fig. 3.5 as a Ω_{RVE} with the PBC applied to a simplified mesh.

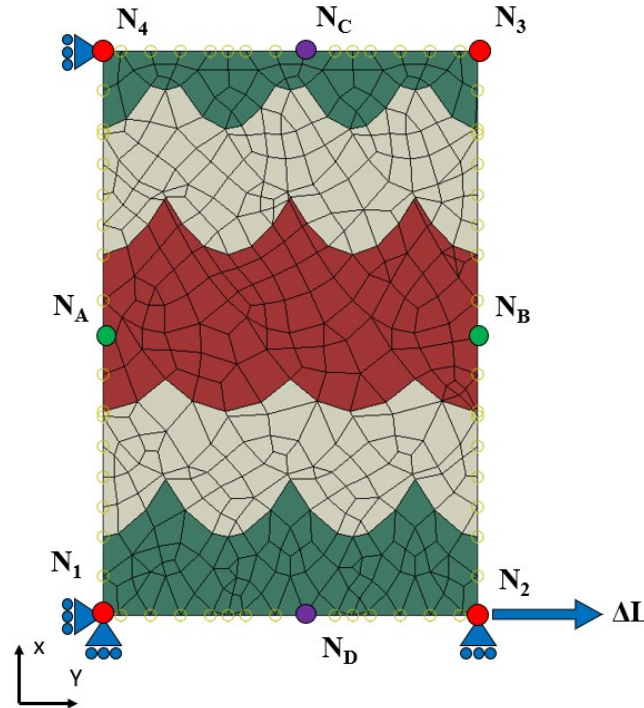


Figure 3.5: Example Abaqus geometry domain created with custom Python script. Periodic boundary conditions (PBC) are applied according to Eq. 3.4 and Eq. 3.5 below to create a representative volume element of the melt pool structure. The mesh nodes at the MPBs and apposing periodic edges are compatible.

The PBC is applied to the Ω_{RVE} following the formulation presented by Kouznetsova et al. (2001) [66], in which the periodicity of Ω_{RVE} is enforced by the kinematic constraints between apposing edges based on the canonical equations of Eq. 3.4 and Eq. 3.5 below.

$$U(x, y)^{N_B} - U(x, y)^{N_A} - U(x, y)^{N_2} + U(x, y)^{N_1} = 0 \quad (3.4)$$

$$U(x, y)^{N_C} - U(x, y)^{N_D} - U(x, y)^{N_4} + U(x, y)^{N_3} = 0 \quad (3.5)$$

The canonical equations relate the x and y displacements, $U(x, y)$, of a given edge node, such as N_A , to the periodically linked compatible node N_B and the corner nodes N_1 and N_2 . Loads are applied to the corner nodes, such as N_2 , which effectively applies the load to the entire edge of the domain. Rigid body motion is prevented by the boundary conditions applied to the corner nodes.

A global mesh size of 5 μm was used for the geometry domains tested here averaging about 200 μm by 300 μm in size. This mesh size was chosen due to the insensitivity of the measured stress and displacement at several selected points within the domain with changes in the global mesh size. Increasing and decreasing the selected global mesh size from 5 μm was found to affect the simulation results by less than 10% difference. In the examples presented in this study, the melt-pool geometry inputs and FGM distributions are chosen so that the generated melt pool structures are inherently periodic, meaning that the application of PBCs to the RVE is very easy and does not create any discontinuities in the results due to mesh or material incompatibilities. Therefore, the size of the RVE is chosen so that one entire unit cell is represented along both the x and y directions, and in these examples, additional repeating sections are included along the x direction to improve the clarity of the results.

The results of the mesoscale simulation are used to estimate the effective material properties of the macroscale part by calculating the volume averaged stress according to the displacements and reaction forces experienced by the corner nodes according to Eq. 3.6 below.

$$\langle \sigma \rangle = \frac{1}{V} [\mathbf{x}_1 \otimes \mathbf{f}_{N_1} + \mathbf{x}_2 \otimes \mathbf{f}_{N_2} + \mathbf{x}_3 \otimes \mathbf{f}_{N_3} + \mathbf{x}_4 \otimes \mathbf{f}_{N_4}] \quad (3.6)$$

The volume averaged stress is denoted by $\langle \sigma \rangle$, V is the total volume of the RVE and $\mathbf{x}_n \otimes \mathbf{f}_{N_n}$ is the tensor product of the displacement and external force at the n^{th} corner node. The full derivation is provided by Okereke and Akpoyomare (2013) [67] and is well suited for small displacements of elastic or strain hardening materials, but represents local response phenomena poorly due to volume-averaging. The effective global strain of the RVE is similarly calculated from the displacement of the corner nodes and the results are used to plot an effective stress-strain curve for the structure and estimate the effective elastic modulus and yield point.

Experimental results from Feng et al. (2017) [68] and others show that for metallic materials with comparable strain hardening behavior, the rule of mixtures (ROM) can accurately estimate the mechanical behavior of the composite material. It is suggested that interface characteristics can be ignored, especially for interfaces of

relatively small thickness, and is tested here by using the rule of mixtures to estimate the effective elastic modulus and yield strength of the structure. The area percentage of each material is measured and used along with the input material elastic modulus or yield strength according to Eq. 3.7 and Eq. 3.8 below to estimate the mechanical properties of the bulk structure in the x and y direction respectively.

$$E_x = \sum \alpha_n E_n \quad (3.7)$$

$$E_y = \left(\sum \frac{\alpha_n}{E_n} \right)^{-1} \quad (3.8)$$

Here, the area percent composition of the n^{th} material is denoted by α_n , E_n represents the elastic modulus or yield strength of the n^{th} material and the E_x and E_y values represent the estimated modulus or yield strength in the x and y directions respectively.

3.4 Test Cases

Three test cases are presented below to show some of the capabilities of the melt pool structure generation tool developed here, and to quantify the effect of different melt-pool geometries of the results of a relatively simple FEA tensile test. There are many possibilities available for melt-pool geometries, melt-pool geometry distributions, material definitions, material definition distributions, loading cases, and much more using this melt pool structure generation tool, and only simplified structures and simulation models are used here to show some of the capabilities. Table 3.2 below highlights some of the characteristics of the three FGM melt pool structures analyzed in the following sections.

Table 3.2: Summary of the test conditions used in the FEA examples in the following sections.

Section	Number of Materials	Material Definition	MP Structure	Boundary Conditions	Loading
3.4.1	2	Ramberg-Osgood	acute and obtuse MPBs	PBC	20% true strain
3.4.2	3	from test data	from samples	PBC	30% true strain
3.4.3	3	from cell structure simulation	from samples	PBC	8% true strain

3.4.1 Comparison of Multiple Melt-Pool Geometries

The effect of local stress and strain concentrations near the layer-layer MPB interfaces between dissimilar material definitions are examined using the melt pool structure shown below in Fig. 3.6a. The structure has a stiff and soft material with different melt-pool geometries to form layer-layer MPBs with obtuse and acute angles, as shown by the red angle indicators. The same PBC described above in section 3.3 is applied to the domain and the material properties are defined according to the Ramberg-Osgood engineering stress vs engineering strain curves shown in Fig. 3.6b. The material property definitions are input into Abaqus as true stress and true strain using the elastic plastic material model discussed in section 3.3. Two different test cases are examined for

this structure. Test case one assigns the stiff Material 1 to the white layers in the middle of the structure, while for test case two, the outer green layers are assigned as the stiff Material 1. Displacements of 20% true strain are applied in the x then y direction for both test cases, for a total of four tests.

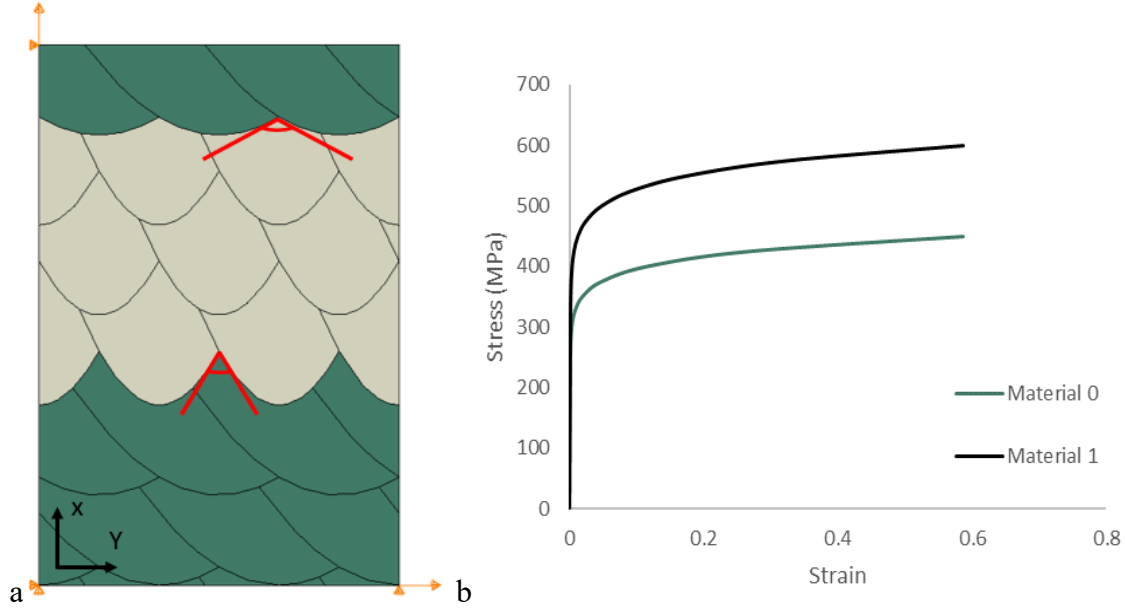


Figure 3.6: A simple two material structure used to investigate the MPB geometry effects between stiff and soft materials. The melt pool structure with boundary conditions and material definitions is shown in a along with the highlighted acute and obtuse angle MPBs. The Material 0 and Material 1 engineering stress vs engineering strain response is given in b.

The von Mises stress and max in-plane principal strain fields of test case one loaded in the x direction are shown below in Fig. 3.7. As expected, the stiffer centrally located Material 1 measures the highest average stress and the lowest average strain when compared to the softer Material 0, indicating that the stiffer material is carrying a larger proportion of the total force applied to the structure. The areas of highest von Mises stress and max in-plane strain are circled in the stress and strain fields. Large stress and strain gradients are observed at the lower acutely angled layer-layer MPB interface where there is significant overlap between the dissimilar materials. The stress gradient even extends past the material overlap and into the center of the melt pool as highlighted in Fig. 3.7. In comparison, the obtuse angled layer-layer MPB near the top of the structure features much smaller stress gradients which is favorable to preventing localized crack formation and failure.

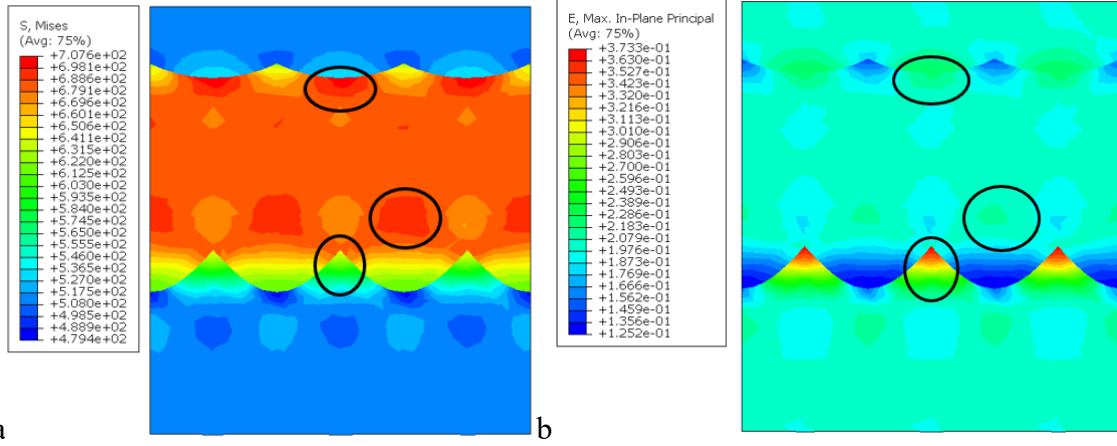


Figure 3.7: The a) stress and b) strain fields of the test case one melt pool structure from Fig. 3.6 above loaded to 20% true strain in the x direction. Interesting local features of the stress and strain fields are highlighted.

The results of test case one loaded in the y direction are shown below in Fig. 3.8. Stress concentrations can be seen in different areas than that from the x-direction loading, and in general, the x displacement test reveals a more uniform stress magnitude within each material compared to that of the y displacement test case. The maximum von Mises stress of the stiffer Material 1 is located near the center of the melt pool, away from the MPB, and covers a relatively large area. The area of highest stress in the softer Material 0 is located near the rounded bottom of the MPB and is also spread over a relatively large area. This is in contrast with the x direction results which showed a local stress minimum in this area. The stress in Material 0 near the acute angled MPB is also very different, with the x direction test showing a local stress maximum and the y direction test showing a local stress minimum. The reduced stress of the y-direction test case within the acute corner is expected to help prevent local failure initiating at the MPB [12].

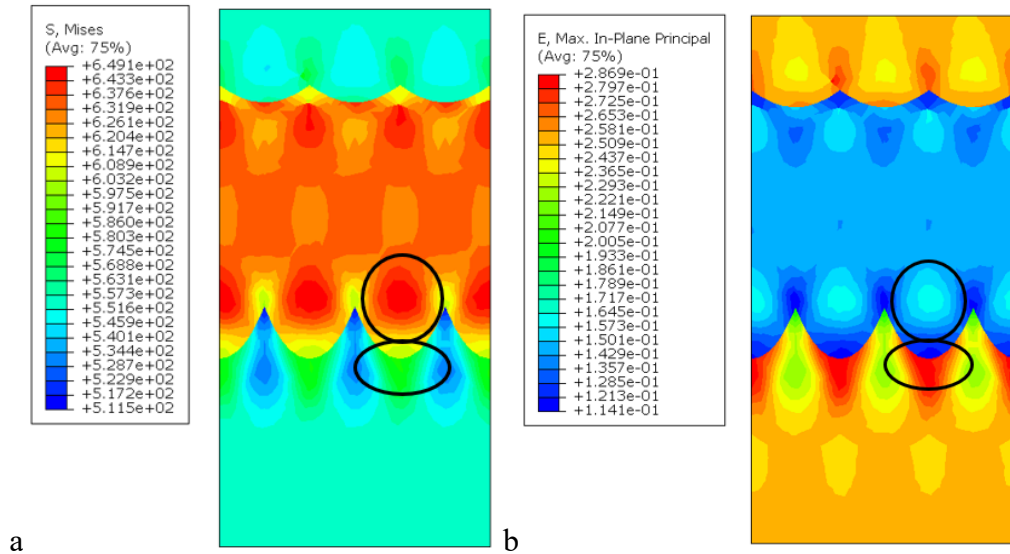


Figure 3.8: The a) stress and b) strain fields of the test case 1 melt pool structure shown in Fig. 3.6 above loaded in the y direction to 20% true strain. Interesting results near the lower layer-layer MPB are highlighted.

The stress and strain fields of the second test case, with the softer material located centrally within the structure, loaded in the x direction are shown in Fig. 3.9 below and

reveal that the areas of maximum stress in both materials occur in the same area of the MPB. In the obtuse angled MPB, the stress concentration is found within the corner of the layer-layer MPB, while for the acute angled MPB, the stress concentration is seen near the rounded area of the layer-layer MPB. These local stress concentrations occurring in both materials across a MPB is likely to increase the risk of local failure beginning within the layer-layer MPB where failure typically occurs according to experimental results from Shifeng et al. (2014) [12].

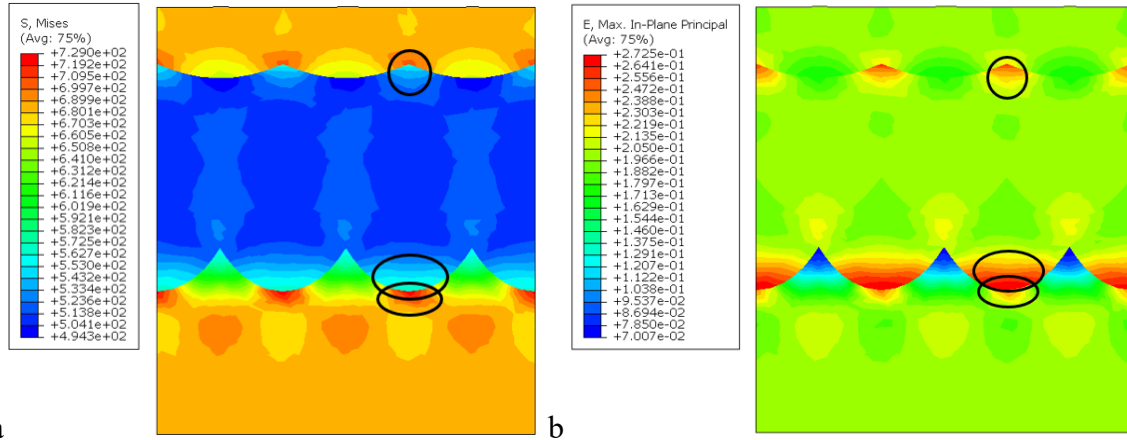


Figure 3.9: The a) stress and b) strain fields of the test case 2 melt pool structure shown in Fig. 3.6 above loaded in the x direction to 20% true strain. Interesting results near the dissimilar material interfaces are highlighted.

Similar to the x direction load applied to test case two, the stress and strain fields of test case two loaded in the y direction in Fig. 3.10 below shows a common stress concentration location for both the stiff and soft materials across the layer-layer MPB. The stress concentration of the y-direction load case is located near the small area near the corner of the acute angled layer-layer MPB. This stress concentration is more localized, measuring a higher concentration factor, and presents a high risk for local failure at the MPB.

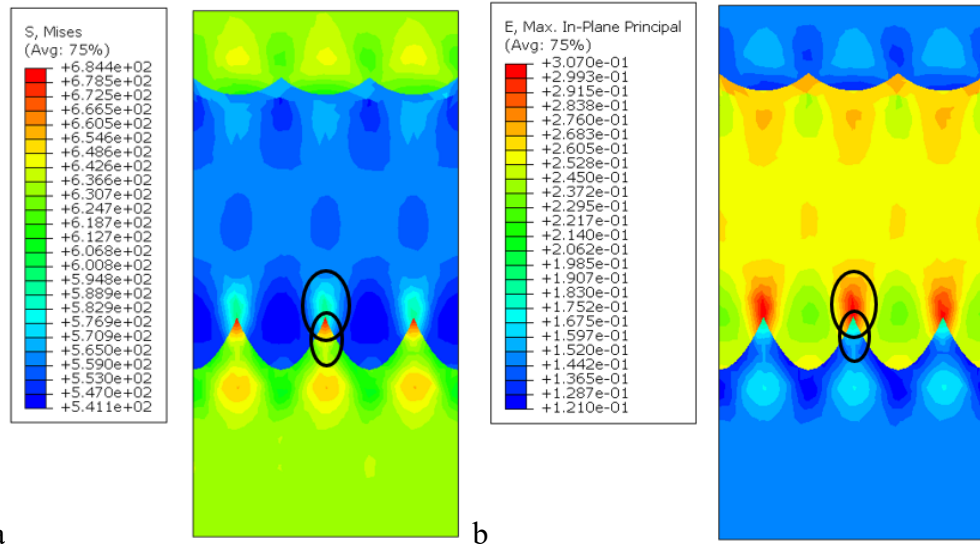


Figure 3.10: The a) stress and b) strain fields of the test case 2 melt pool structure shown in Fig. 3.6 above loaded in the y direction to 20% true strain. The areas of maximum stress in each material are highlighted.

The volume averaged effective stress and strain response of test cases one and two loaded in the x and y directions are plotted below in Fig. 3.11 along with the Ramberg-Osgood stress strain curves of the soft and stiff materials. According to the volume averaged stress and strain results, the bulk plastic response of both structures loaded in both the x and y direction are similar. This is because the volume averaged response is highly dependent upon the input material properties.

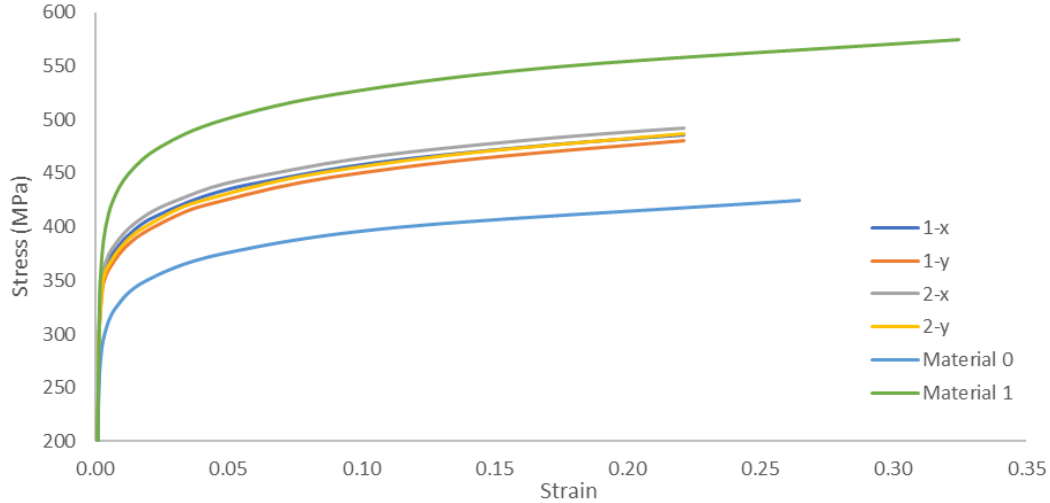


Figure 3.11: Plot showing the volume averaged effective engineering stress vs engineering strain response of all four test cases of the melt pool structure shown in Fig. 3.6. The engineering stress vs engineering strain responses of Material 0 and Material 1 are also plotted for reference.

The effective yield point and stress within the plastic deformation region of the structure is very close to midway between the properties of the soft and stiff materials making-up the structure. In Table 3.3 below, the measured elastic modulus and yield stress of each test condition are given, as well as a comparison of the measured mechanical properties with the properties estimated by the ROM method.

Table 3.3: The measured elastic modulus and yield stress of the example melt pool structure for both the x and y-direction test cases. The results of the rule of mixtures estimated elastic modulus is also shown with the percent difference comparison to the measured value.

Test Case	Measurements		Rule of Mixtures		% Difference	
	Modulus (GPa)	Yield Stress (MPa)	Modulus (GPa)	Yield Stress (MPa)	Modulus (GPa)	Yield Stress (MPa)
1-x	189.943	360.63	194.781	347.81	2.547	3.556
1-y	194.591	352.46	194.653	340.73	0.032	3.330
2-x	195.184	366.16	195.219	352.19	0.018	3.815
2-y	195.039	357.16	195.091	345.02	0.027	3.400
Material 0	190.000	300.00				
Material 1	200.000	400.00				

There is less than a 4% difference between the measured and ROM estimated properties of the tested structures. Interestingly, test case 1 loaded in the x direction

measured the lowest elastic modulus and had the least accurate estimated modulus using the ROM compared to the other test conditions. One possible explanation for this lower-than-expected modulus measurement is that the lower layer of the stiffer centrally located material is limited by the soft material below where they overlap. In this area of melt pool overlap, the soft material prevents the stiff material from carrying a substantial portion of the stress which effectively reduces the total percent area composition of the stiff material for this test case.

The yield strengths of each test condition estimated by the ROM are similar in accuracy to the measured values. The measured yield strength is about 3.5% higher than the ROM prediction, but these results suggest that the ROM can accurately estimate the elastic modulus and yield strength of melt pool structures with simple Ramberg-Osgood material definitions.

3.4.2 Material Definitions from Test Data

To analyze the response of realistic SLM manufactured materials and structure geometries, a melt pool structure was created using the measured tensile stress response and observed melt-pool geometry of the three different dog bone sample groups created. Geometry parameters used to create the melt pool structure were selected to match the SEM imaged melt-pool geometries of the samples and the resulting melt pool structure can be seen in Fig. 3.12a below featuring three unique sections, each with four layers. The elastic plastic material response was chosen to match that of the tensile test DIC data for the three different sample groups shown below in Fig. 3.12b.

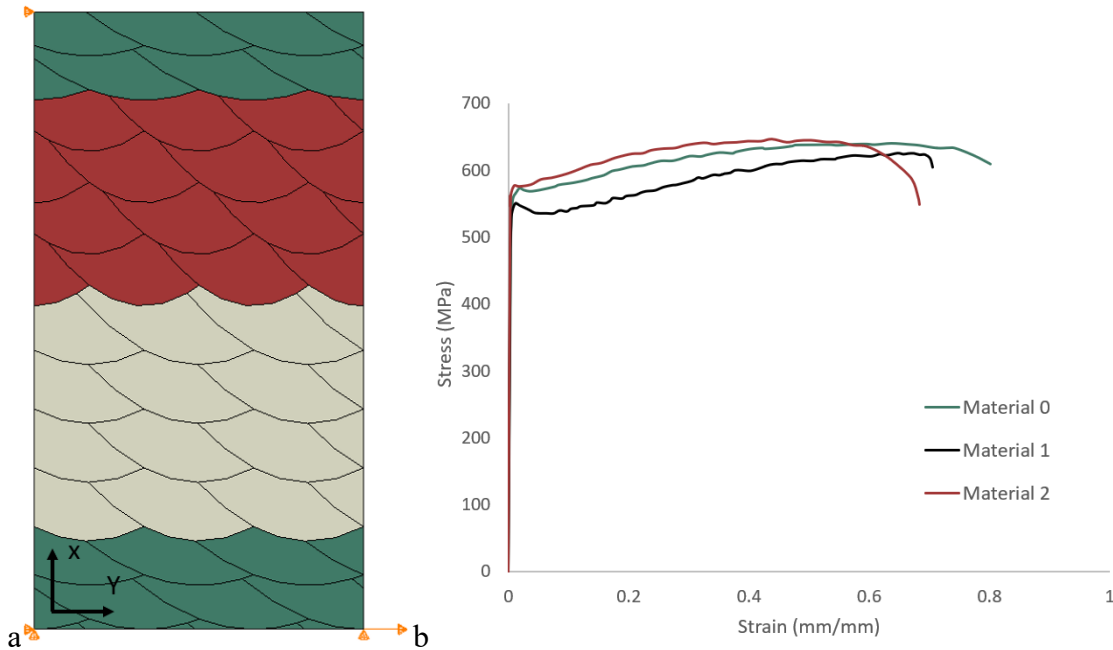


Figure 3.12: a) Melt pool structure with geometry and b) tensile engineering stress vs engineering strain response of the prepared dog bone samples measured with DIC. Material 0, 1 and 2 represent sample groups 2, 3 and 1 respectively.

The structure was tested with an x and then y direction tensile displacement of 30% true strain and PBCs were applied to all four edges of the domain. The stress and strain fields of the x-direction test case are given in Fig. 3.1 3 and clearly show the

difference in relative stiffness of the materials. The stress and strain magnitudes are relatively constant throughout each of the materials of the structure except in small, localized areas. The main stress concentration is observed near the middle of the domain at the dissimilar material interface between the stiffest Material 2 and the softest Material 1 and is located across the MPB which makes this area very susceptible to local failure according to experimental results from Shifeng et al. (2014) [12].

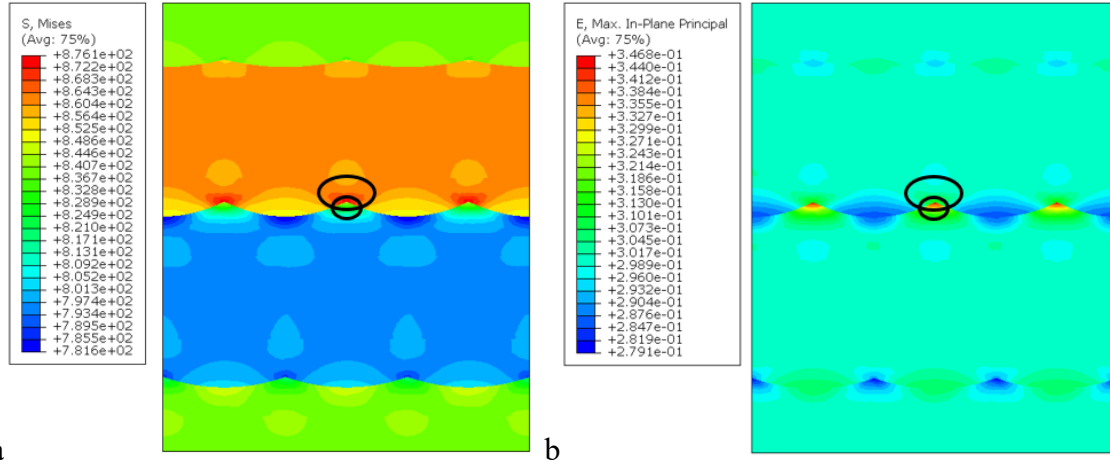


Figure 3.13: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.12 above loaded in the x direction to 30% true strain. The areas of maximum stress are highlighted.

The y-direction test case results are shown below in Fig. 3.14 and reveal stress concentrations near the layer-layer MPB between the stiffest Material 2 and the softest Material 1 similar to the x direction results. The high stress areas in both materials are relatively large which helps to limit the magnitude of the stress concentration. The high stress area in the stiffest material is also offset slightly from the MPB, removing the concentrated stress from the likely failure area. Like the results from test case one for the previous structure above, the stress concentration in the x-displacement test case is found near the corner of the MPB, but the stress concentration in the y-direction test case is located near the rounded area of the MPB. This similarity is likely due to the stiffer material being located above the softer material, because test case two of the previous structure has the opposite stiff and soft material order and the locations of the stress concentrations in the x and y direction test conditions are reversed.

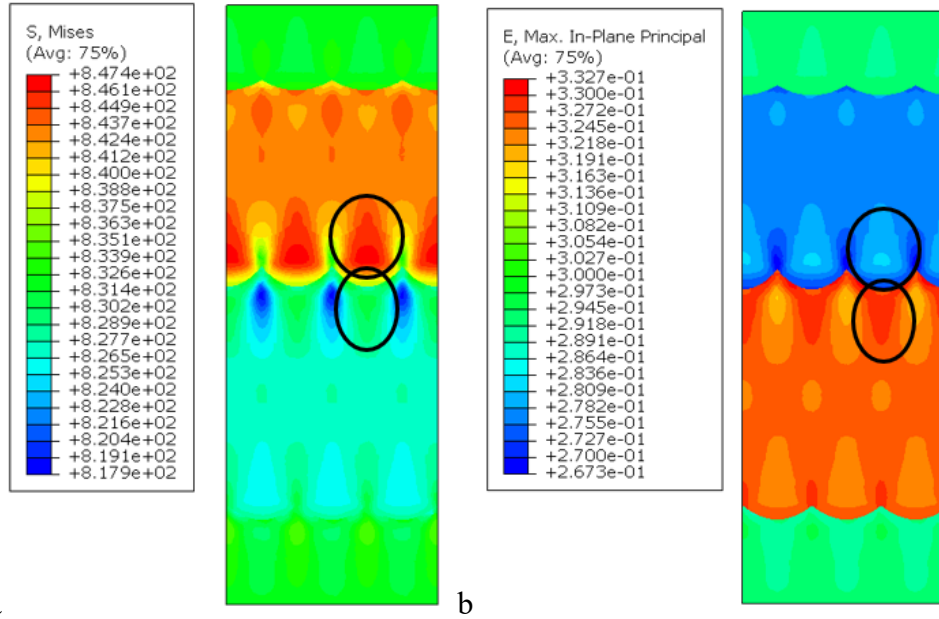


Figure 3.14: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.12 above loaded in the y direction to 30% true strain. The areas of maximum stress are highlighted.

The volume averaged effective stress and strain responses of the structure tested in both the x and y direction are plotted in Fig. 3.15 along with the original material definitions from the DIC test data. The effective stress and strain curves closely follow the average of the input material parameters as expected.

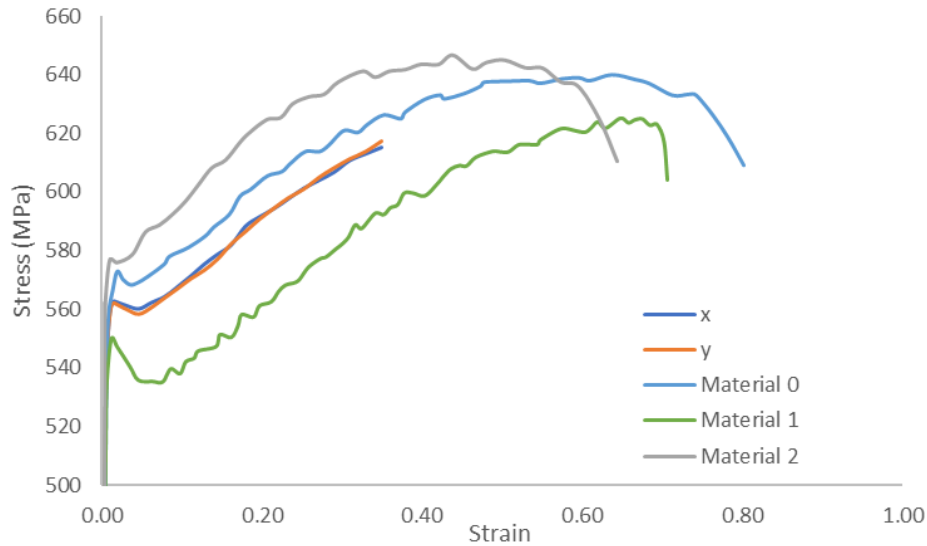


Figure 3.15: Plot of the volume averaged effective engineering stress vs engineering strain response of the melt pool structure. Both the x and y direction results are plotted with the tensile responses of the three sample groups for reference.

As shown by the results in Table 3.4, the ROM is again accurate in predicting the elastic modulus of the tested structure to within 2% difference. This test also provided a good estimate of the yield strength, most likely due to the smaller amount of overlap between the dissimilar layer interfaces. Again, the x-direction test case shows a higher

percent difference between the FEA measured and ROM predicted elastic modulus than the y-direction test case, similar to test case one for the previous structure. This similarity in the ROM predicted modulus inaccuracy is likely related to the similarity in the stress field of both test cases.

Table 3.4: Volume averaged effective elastic modulus and yield strength measured for both tensile loading conditions. The rule of mixtures estimated modulus and its comparison to the measured values are also given.

Test Direction	Measurements		Rule of Mixtures		% Difference	
	Modulus (GPa)	Yield Stress (MPa)	Modulus (GPa)	Yield Stress (MPa)	Modulus (GPa)	Yield Stress (MPa)
x	137.948	562.93	138.221	565.32	0.198	0.424
y	135.925	562.37	135.926	565.04	0.001	0.475
Material 0	115.551	572.91				
Material 1	135.659	549.76				
Material 2	160.877	577.03				

3.4.3 Performance Prediction from Cell Geometry

Using the simulation framework created by Moneghan et al. (2020) [69], a multiple length-scale analysis is performed, beginning with an inspection of the cell structure. SEM images of the cellular structure of each sample group were used to create a 2-dimensional Abaqus model to measure the effective stress-strain response of the cellular microstructure. The Abaqus results were used as material definition inputs for the mesoscale melt pool structure simulation previously defined. The melt-pool geometry is based on SEM images of the test samples to replicate the melt-pool geometry. The performance prediction from cell geometry example in this section is used to show the general process of applying homogenize effective stress results from a micro scale FEA simulation to the materials used in the generated melt pool structure FEA simulation. The simple modeling methods used here are not expected to produce highly accurate estimates of the part mechanical performance but show one method by which the melt pool structure generation tool created here can be paired with simulation results from other studies.

SEM images of the cells of the three sample groups are processed by a custom trained U-Net CNN to segment the image pixels containing cell boundaries from the cells. The segmented image is then input into Abaqus to provide model geometry created directly from the physically observed structure, as shown in Fig. 3.16. The exact mechanical properties of the cells and cell boundaries are unknown, but due to the increased concentration of nickel, chromium and molybdenum as well as the BCC crystal structure in the cell boundaries, this material is estimated to be stiffer and stronger than the cell material according to Moneghan et al. (2020) [69].

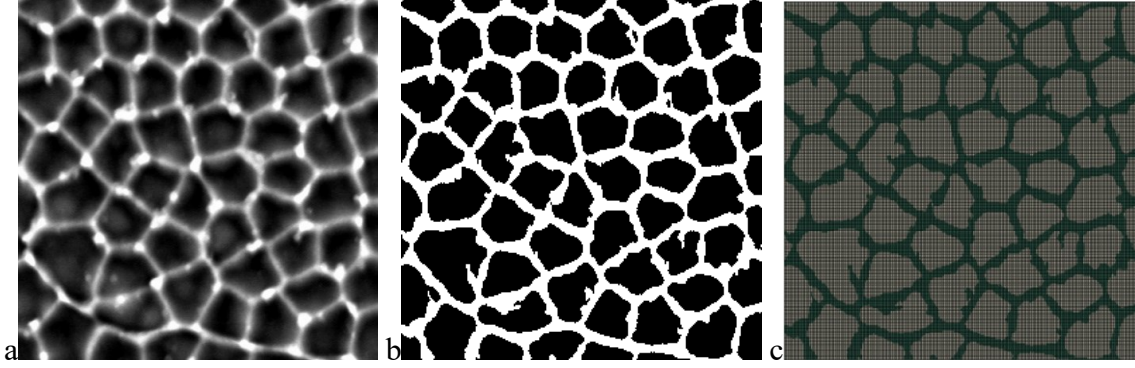


Figure 3.16: Process of converting a) section of raw SEM image to a b) a binary image separating the cell and cell boundary materials to be imported into Abaqus as a c) meshed geometry domain using a custom Python script.

To mimic the cell and cell boundary materials, the mechanical properties of conventionally manufactured 316L and 4340 steels provided by *Materials Science and Engineering and Introduction* [70] and *Mechanical Behavior of Materials* [71] are used respectively, similar to what was done by Moneghan et al. (2020) [69]. The test geometries representing each of the sample groups are shown below in Fig. 3.17.

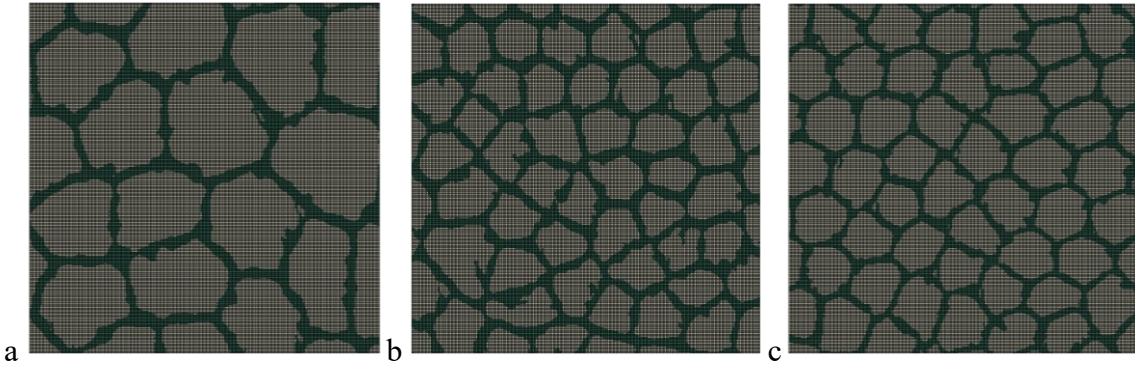


Figure 3.17: Abaqus models of the sample group a) 1, b) 2 and c) 3 cellular structures imaged by SEM.

As evident by the SEM images and the cell size analysis discussed earlier, the cells of sample group 1 are significantly larger than those of groups 2 and 3. The differences between the cells of groups 2 and 3 are less notable, but it is observed that the cell boundaries of the group 2 specimen are slightly thicker than that of group 3. Resulting in a higher percent area composition of the stiffer cell boundary material in group 2 (32.50%) compared to group 3 (27.02%) and group 1 (22.28%).

A tensile displacement of 10% true strain was applied in the x then y direction separately to each geometry. The 2D cell structures tested were found to have an isotropic stress response, as expected. The difference between the x and y direction stress responses were very small, measuring less than 1.5% difference in stress for any given strain measurement. For this reason, only the x direction tensile results are presented below in Fig. 3.18, which are representative of any test direction.

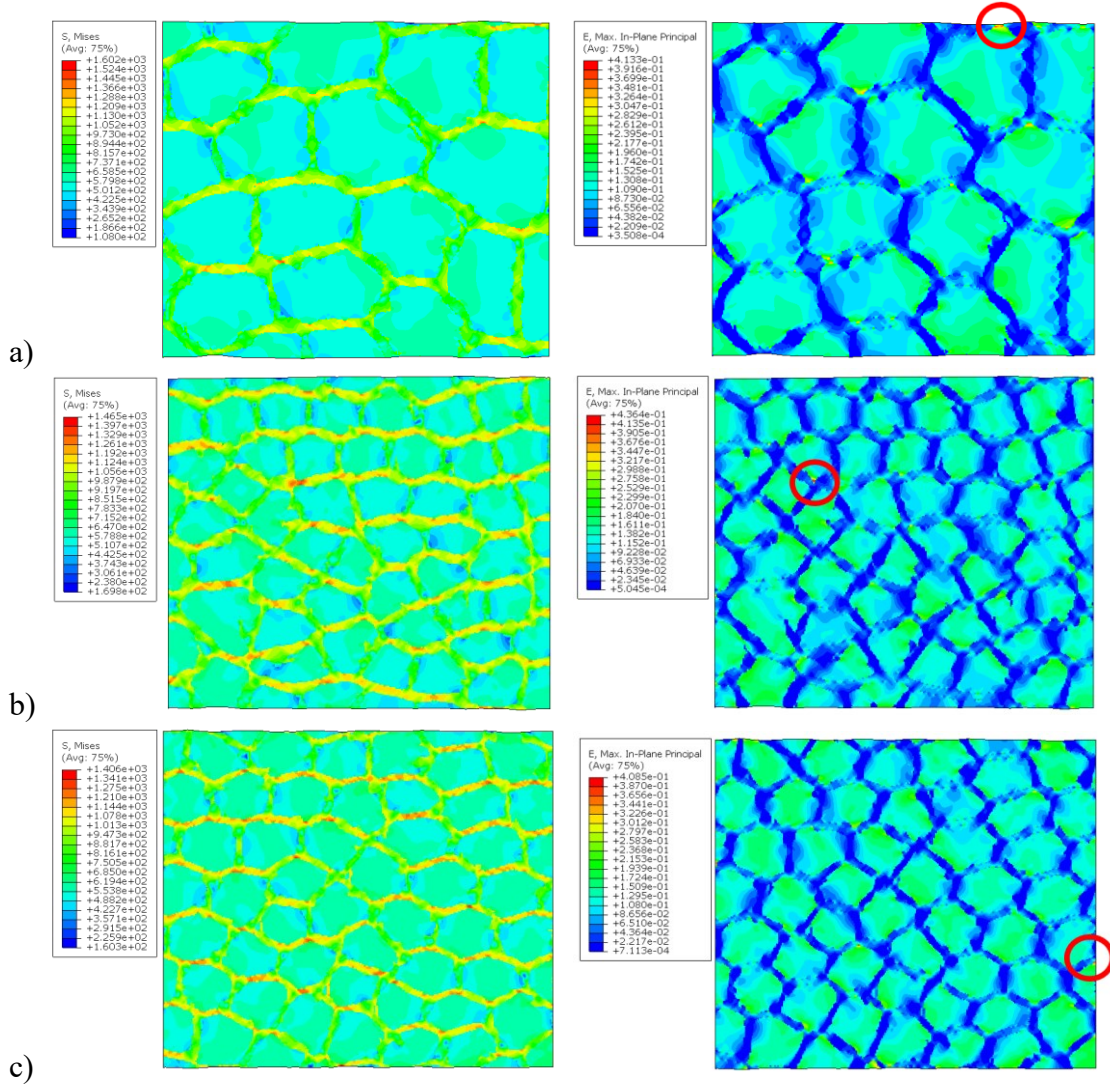


Figure 3.18: The stress and strain fields of the a) group 1, b) group 2 and c) group 3 sample cell structures loaded to 10% true strain. Locations of local strain concentrations have been highlighted with red circles.

Overall, the stress and strain fields of the three test structures in Fig. 3.18 appear very similar. The areas of highest stress concentrations are found in the stiffer cell boundary material as expected. More specifically, the stress concentrations are mostly found in horizontal lengths of cell boundary material because the domain is loaded along the x direction. The strain fields show a mostly consistent separation of strain magnitude between cell and cell boundary materials due to the stiffness mismatch. Strain concentrations are isolated to very small areas within the cell material located near the inside of corners created by the cell boundary material and near or at the domain edge. The strain concentrations are located in these areas because of the stress concentration or discontinuity in the stiffer load bearing cell boundary material. The small section of soft material surrounded mostly by stiff material creates a large strain concentration in the soft material and is an area at risk of local failure. This suggests that the discontinuities in the cellular structure observed near grain boundaries and MPBs are also locations likely to have strain concentrations and susceptible to local failure. This aligns with the simulation and experimental findings of Moneghan et al. (2020) [69] and Shifeng et al.

(2014) [12] respectively which showed that crack growth preferentially grows along the MPBs rather than through the cellular structure. The fatigue simulation results provided by Ghodrati and Mirzaeifar (2020) [50] also showed that strain concentrations in similar areas of the cell material near the cell boundary material measured the highest accumulated damage, supporting that these areas are the most likely points of failure within the uninterrupted cell structure.

The effective stress responses of the three different sample group structures are shown below in Fig. 3.19. The effective stress is given as the volume averaged stress, calculated by integration of the stress measurement at each point in the domain. This is similar to the result of the volume averaged stress formula of Eq. 3.6, but is applicable to the non-periodic geometry domain used here.

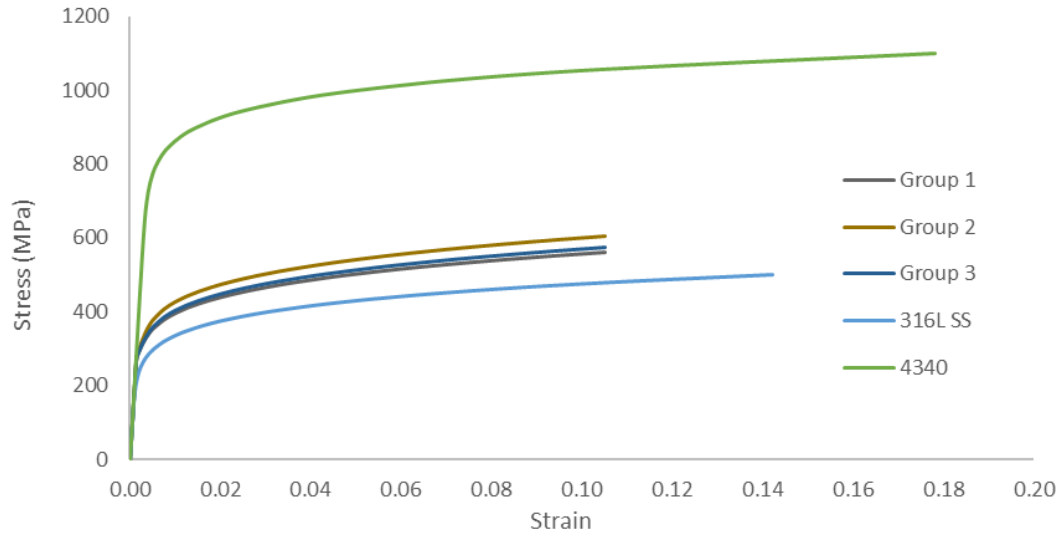


Figure 3.19: The effective stress response of the cellular microstructures of the three sample groups is plotted along with the 316L and 4340 steel input material properties for reference.

The stress response results plotted in Fig. 3.19 above and the mechanical properties given in Table 3.5 below show that the group 2 material measured the highest stiffness and yield strength. The small cell size and relatively thick cell boundaries of the group 2 cell structure improved the yield strength over the large cells of group 1 and the thinner cell boundaries of group 3. This is consistent with expectations and the findings of Moneghan (2020) [49], where the combination of thicker cell boundaries and smaller more tightly spaced cells were found to produce the cell structure with highest yield strength in a cell geometry optimization study.

Table 3.5: Volume averaged effective elastic modulus and yield strength measured for each sample group cellular structure. The percent area composition of the stiffer 4340 steel is also shown for comparison.

Test Case	Elastic Modulus (GPa)	Yield Stress (MPa)	% Composition 4340
Group 1	195.822	333.60	22.28
Group 2	197.243	355.11	32.50
Group 3	196.467	336.56	27.02
316L SS	192.800	275	
4340	207.000	800	

The measured properties of each tested cell structure were used as material definition inputs to represent each sample group. The same melt pool structure previously created to represent the geometry of the observed melt pools in each sample group is reused here with the new material definitions. The reused melt pool structure and the new material definitions are shown below in Fig. 3.20.

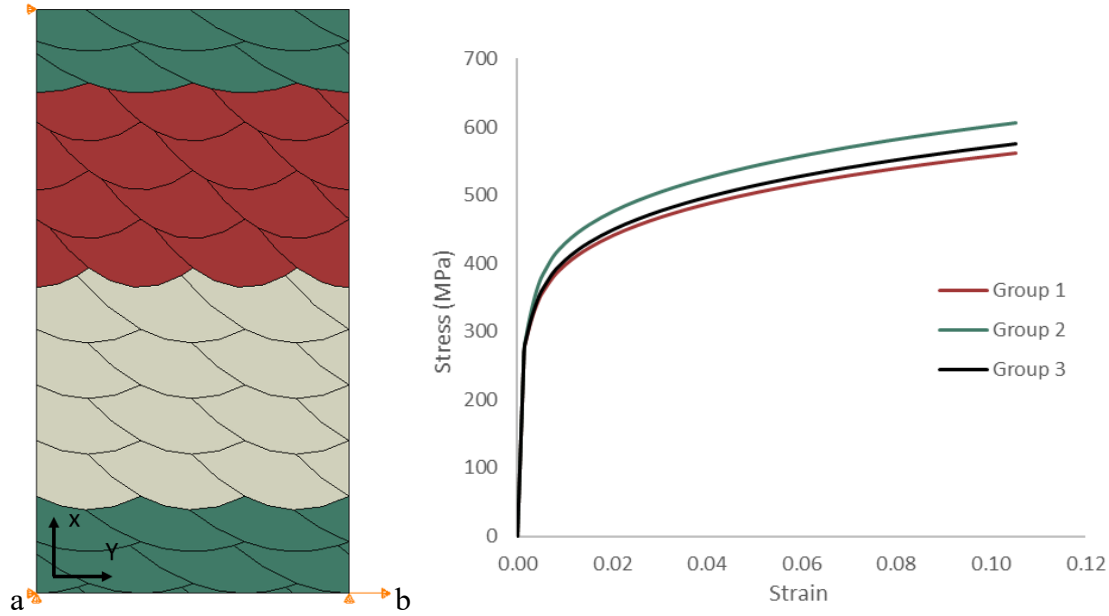


Figure 3.20: a) Gradient melt pool structure representing the observed melt-pool geometry found in the three different sample groups. This is the same structure as used above, shown in Fig. 3.12. b) The material definitions assigned to similarly colored layers of the melt pool structure, based on the results of the tested cell structures.

The same PBCs were used to create a RVE for testing, and a true strain of 8% was applied in the x and then y direction. The von Mises stress and maximum in-plane principal strain fields of the x direction displacement test are shown below in Fig. 3.21. Both the stress and strain fields show relatively little variation across the domain, mainly because the variation in material properties is small. The strain field reveals the locations of strain concentration at the MPB between the softest and stiffest material as expected.

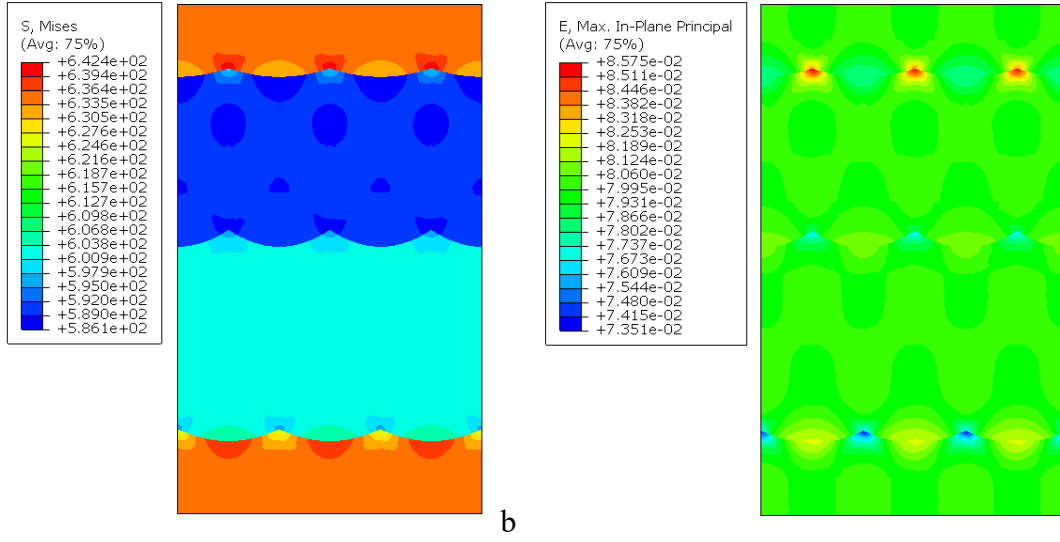


Figure 3.21: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.20 above loaded in the x direction to 8% true strain.

The stress and strain fields of the y direction test are displayed below in Fig. 3.22 and show more variation than the x direction test. The stress and strain concentrations are in about the same locations as in the x direction test above but are more dispersed. In the y direction test, the geometry of the MPBs have a more significant effect on the distribution of stress and strain within the structure. Stress resulting from the Poisson ratio likely contributes to these unique stress distributions.

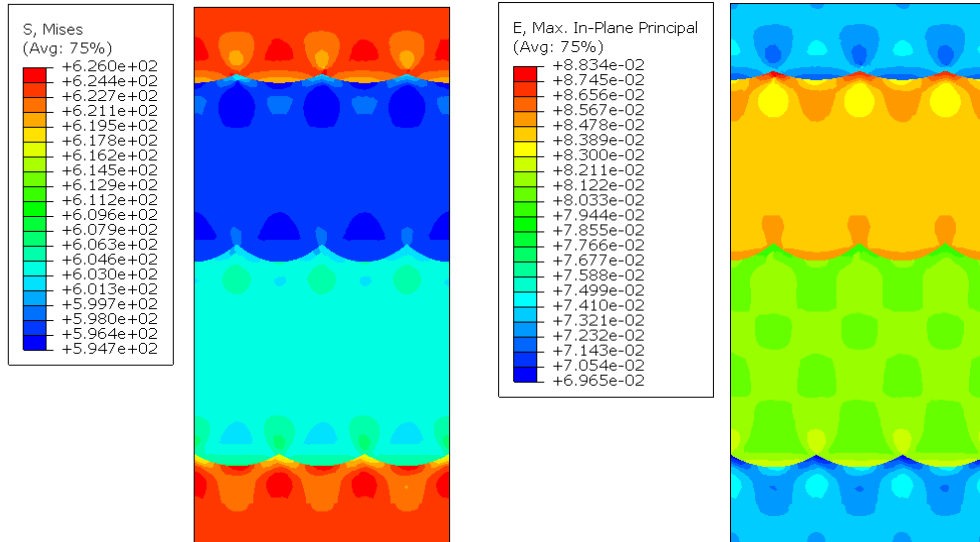


Figure 3.22: The a) stress and b) strain fields of the melt pool structure shown in Fig. 3.20 above loaded in the y direction to 8% true strain.

The stress and strain concentrations observed for both test directions are not large in magnitude or area, but are located almost exclusively near the MPBs, which as discussed earlier, is detrimental to the local yield and ultimate tensile strength. The measured elastic modulus and yield stress of the structure are very similar for both test directions, with the modulus measuring 196.42 GPa and 196.33 GPa for the x and y

direction tests respectively. The similar yield stress measurements, however, measured higher than the yield strength of the input materials, which is not expected. This modeling inaccuracy is due to the yield strength of the input materials being estimated via the 0.2% strain method and used to create the Abaqus elastic-plastic curve for two consecutive simulations.

The Abaqus elastic plastic material model assumes a perfectly linear elastic region until yielding, and tabulated values are used to define the plastic region. In this study, the yield point is determined using the 0.2% offset method for consistent yield measurements.

Using the 0.2% offset method, some of the smooth transition area between the elastic and plastic regions until the yield point is straightened to create a perfectly elastic region in Abaqus. This creates a discontinuity in the slope of the Ramberg-Osgood elastic plastic stress vs strain curve input into Abaqus and is expected to slightly overestimate the yield stress and underestimate the strain at yield, by only a few percent difference. When the results of the cell structure analysis are used as inputs for the melt pool structure materials, the 0.2% offset method is applied to the stress vs strain curve a second time, compounding upon the overestimated field stress and underestimated yield strain. The compounded error creates a larger observable discontinuity in the stress vs strain slope at the yield point, essentially turning the smooth Ramberg-Osgood curve into an elastic plastic curve with an instantaneous transition.

3.5 Microstructure Modeling Results and Discussion

The FEA results showed that the homogenized stress-strain responses were highly dependent upon the percent material composition of the structure, similar to composite materials. The ROM provided accurate elastic modulus and yield stress estimates for most tests, measuring less than 4% difference between the FEA homogenized results and the ROM predictions. The highest stress concentrations were observed near acute angles in the MPBs between dissimilar materials, which is in agreement with experimental failure analysis of similar samples [12]. Specifically, it was observed that acute angled MPBs with stiff material positioned below softer material are likely to create stress concentrations across the MPB for both x and y loading directions. In contrast, obtuse angled MPBs more effectively limited stress concentrations near the MPB for the material and structure combinations tested. For the same materials, the acute MPB geometry measured about 14% higher von Mises stress than the obtuse geometry.

As expected, it was clear to see the differences in material stiffness due to the amount of stress carried by the material, and the areas of stress concentrations were observed near the dissimilar material interfaces. Some stress concentrations were also observed away from the MPBs, towards the center of the individual melt pools, which was likely a result of geometric effects from the MPB.

Based on the work conducted by Moneghan (2020) [49], it was observed that the yield strength and stiffness of the cellular structure is highly dependent on the amount of the stiffer cell boundary material. To properly incorporate the results from the cell structure length scale to the proposed melt pool structure model, a different homogenization method or material model should be used to avoid the inaccurate elastic to plastic transition zone of the effective material response observed here.

The test cases presented here are not necessarily useful for measuring the performance of SLM parts directly but show some of the capabilities of the melt pool creation tool and Abaqus scripts developed here. Unique melt-pool geometries were created to represent each of the three fabricated specimen groups in sections 3.4.2 and 3.4.3. In section 3.4.1 two very different melt-pool geometries were created to achieve different layer-layer MPB geometries. Altering the melt-pool geometries was also shown to have a measurable effect on the local stress and strain distribution as well as the homogenized stress vs strain response of the structure.

The melt pool structure generation tool developed here is applicable to the creation of most melt pool geometries typically observed from SLM parts created using a single laser scanning direction. Most combinations of input values such as the width, height and shape described in Section 3.2 defining the melt pool geometries will successfully generate a melt pool structure. In most cases, any structure generation failures are caused by too large of a change in any single or multiple input values such as height, width and shape between neighboring melt pools. In other cases, it is possible to resolve structure generation failures by slightly changing the input values. The current tool is only able to create melt pool geometries representative of melt pool structures created by using a single laser scan direction because the geometry is 2-dimensional. The tool is also best suited for creating a periodic repeating structure due to the ease of using the PBCs.

The melt pool geometry creation tool is intended to be used in conjunction with simulation methods developed in other studies to improve the simplified semi-circle geometry leading to more accurate results to investigate the mechanical performance of SLM parts. The results obtained here have provided evidence that the melt pool structure geometry is relevant to the mechanical performance of SLM parts and that the tool developed here can create realistic melt pool structures, including FGM structures, to be paired with more advanced simulation methods.

4 Conclusions and Future Work

4.1 Summary and Conclusions

The advancement of additive manufacturing (AM) technologies is expanding capabilities for more complex part geometries, the reduction in manufacturing costs, the creation of unique functionally graded materials (FGMs) and more. To accommodate the rapidly growing AM capabilities, improvements must be made to the quality assurance and testing of AM parts. In this study, new tools are introduced for the automated analysis of microstructure features from optical and scanning electron microscopy (SEM) images to characterize AM part manufacturing quality and mechanical performance. The developed tools use existing image analysis methods to greatly reduce the time and effort required to characterize AM part microstructures with little to no cost in estimated accuracy compared to traditional methods. A custom melt pool structure generation tool is also developed to improve some of the existing mechanical performance estimation studies by allowing for the simple creation of complex representative melt-pool geometries.

The main contributions of this work are the three tools listed below, which have been developed here to aid in the characterization and virtual testing of selective laser melted (SLM) AM parts.

- (1) A Python script for the automatic processing and evaluation of optical images for quantitative defect content characterization. The metrics of defect sizes and number of defects are output and post processed.
- (2) A custom Mask R-CNN object segmentation model was trained and evaluated for the segmentation of sub-granular cell geometries from SEM images for cell size and morphology analysis.
- (3) A Python script for creating custom melt pool structures that can easily be loaded into Abaqus for finite element analysis (FEA) modeling with automatically generated periodic boundary conditions (PBCs). The created structures are intended to be easily implemented into workflows of previous studies to improve upon the semi-circle melt pool assumption typically used and to provide a means to easily create and study FGM structures.

The developed tools were used to evaluate three different sets of 316L stainless steel (SS) tensile test specimens created via the SLM AM process with different fabrication processing parameters. A sample from each group of unique fabrication processing parameters was evaluated by capturing microstructure images with optical and SEM microscopes. The first and second image-based material characterization tools developed here were used to quantitatively measure the void content and cell size distributions of the tested samples.

The defect characterization tool presented in this work provides a relatively simple means to automatically measure the content and morphology of SLM processing defects from optical images. The tool produces results with good repeatability for much less cost than higher accuracy methods such as X-ray computed tomography (XCT).

The sample optical images were analyzed with the OpenCV Python library which provided high resolution segmented defect morphologies. A high estimated segmentation

prediction accuracy was achieved, leading to an estimated percent defect content accuracy of $\pm 0.05\%$ points as discussed in section 2.4.2. Much of the measurement uncertainty comes from the validity of the assumption that the imaged cross-sectional area adequately represents the volume of the sample.

The void content was estimated to be less than 0.2% for all samples, indicating good melting and solidification of the powder material and high volumetric part densities. The defect content was closely related to the VED, as reported by previous studies, but in section 2.4.2 was found to be most dependent upon the laser energy used during processing. Both keyhole and lack of fusion voids were observed in every sample. Greater than 50% of observed defects measured $2.045 \mu\text{m}^2$ or smaller, which suggests that the samples are dominated by keyhole voids. A greater amount of lack of fusion voids were found in the group 2 sample compared to the other sample groups because the group 2 sample was processed with the lowest laser power.

The results of the image-based percent defect content measurements correlated well with the part density measurements reported by previous studies. However, the part densities measured by the Archimedes' Principle did not match the image-based defect content measurements or the results of previous studies as expected. The validation of the defect content results predicted by the defect characterization tool created here is therefore inconclusive, and more data is required to assess the accuracy of the defect content results.

The measured material tensile strength from section 2.4.1 was observed to be more closely related to the number of defects present rather than the total defect content as discussed in section 2.4.2. This also supports the importance of imaging methods to analyze sample defect content rather than volumetric density measurements because volumetric methods are not able to measure defect count. The results of section 2.4.2 also suggest that the laser power fabrication processing parameter is more influential than the VED on the resulting microstructure of SLM 316L SS, which contrasts with other similar experimental studies. The defect characterization results also concluded that most of the defects in SLM 316L SS parts manufactured with fabrication processing parameters similar to those tested here are small keyhole voids smaller than $2 \mu\text{m}^2$ in cross-sectional area.

The complex cell structures of the prepared SLM 316L SS samples were analyzed using a custom trained open-source Mask R-CNN object segmentation model to accurately segment cell geometries and characterize the cell size distributions, measured as cell area and primary dendrite arm spacing (PDAS). As described in section 2.3.3, the model training was enhanced with image augmentation and measured low loss statistics, indicating good recognition of cell geometry. The trained model produced accurate segmentation predictions with an average intersection over union (IOU) score of 87.9%. A comparison between the manually annotated validation data and the model predicted data in section 2.4.3 also suggested a high model predicted segmentation accuracy, with only a $0.0021 \mu\text{m}^2$ (1.86%) difference in the measured average cell area. The cell segmentation model predictions are nearly identical to those produced manually by a human operator, and therefore, the model predictions are considered suitable for cell size characterization.

From the cell size data observed here, it was found that increasing the laser power increased the average cell size, which agrees with previous studies examining similar

samples. The group 1 sample, which was manufactured with the highest laser power, measured the highest average cell size as well as the highest standard deviation in cell size. Unlike the conclusions from other studies, no clear trend was identified between cell size and material yield or ultimate tensile strength.

The high segmentation accuracy of the model also supports the viability of computer vision technologies such as Mask R-CNN for use in automating and improving material characterization. The model presented here outputs cell segmentations from sample images three or four orders of magnitude faster than an average human researcher with nearly the exact same accuracy. The task of segmenting and analyzing thousands of images for microstructure characterization, such as cell morphology analyzed here, could be completed in a few minutes rather than tens of hours, increasing the number of images that can be analyzed.

The melt pool structure generation tool developed in this research was shown to be capable of creating unique melt pool structures with fully enclosed melt-pool geometries required for FEA. From a few simple user inputs, the geometry and distribution of melt pools are fully controllable to create observed melt-pool geometries and FGMs. The importance of the melt pool structure geometry in tensile loading was studied using FEA to compare stress concentrations and homogenized stress responses. Different FGM structures were created with simple constituent material stress-strain definitions using Ramberg-Osgood, sample tensile DIC test data and estimations from the sample cell structure.

It was concluded that the melt-pool geometry has a measurable effect on the stress concentrations and stress magnitude at interfaces between dissimilar materials. The results presented in section 3.4 show that the highest stress concentrations were located near acute MPB intersections, with different geometries at the MPB causing a change in the measured von Mises stress magnitude of over 10%. The results also showed that the rule of mixtures is useful in estimating the elastic and yield properties of the structures tested, supporting the findings of previous studies. For the relatively simple static structural tests performed here, the percent difference between the homogenized FEA results and the rule of mixture estimations were less than 4% for both the elastic modulus and the yield strength.

The custom Python scripts used to load the created melt pool structure into Abaqus and automatically create the PBCs also proved to be robust, working properly for all the structures considered here and most of the additional structures created but not presented. The PBCs implemented in previous studies were used here effectively to create representative volume elements to examine the stress response of the melt pool structures with a relatively small geometry domain, requiring less computation time. This is very important for the implementation of this melt pool structure generator tool in more complex material models and computational methods proposed in other studies in which the model size is limited by computational power. It is expected that this tool can enhance the accuracy of the FEA models presented in other studies by creating geometries that are more representative of SLM part structures than the simplified semi-circle geometries commonly used.

4.2 Future Work

Expanding upon the work completed here, there are many areas of interest to try to improve the results and continue to contribute to the characterization and virtual testing of AM parts.

Three key topics of future work are highlighted below as beneficial continuations of the work presented here with the goal to improve the results obtained here and continue to contribute to the characterization and virtual testing of AM parts.

- (1) Acquire more defect measurement data from other measurement techniques to properly validate the volumetric defect content estimated by the image-based defect characterization tool developed here.
- (2) Train the Mask R-CNN model to also identify and segment melt pools from SEM images.
- (3) Apply the melt pool generation tool to create improved melt-pool geometries for FEA models developed in previous studies to quantify the impact of the different melt-pool geometries in more sophisticated simulations.

To properly validate the results of the void content measurement methods and tool presented here, it is necessary to inspect a larger number of samples and compare the results with higher accuracy void measurement techniques. It would also be interesting to add the capability to automatically classify detected voids as either keyhole or lack of fusion voids, similar to how scratches are currently detected and ignored. However, the details that create distinguishable differences between these types of voids are largely removed in the binary segmentations, meaning that it will likely be difficult to produce reliable classification results using the same or similar methods currently used for defect segmentation.

The segmentation accuracy of the Mask R-CNN model could be improved by adding more manually annotated images to the training data set and further training the model. However, this is expected to yield only very small accuracy improvements because the accuracy of the model is already very high. Aside from small improvements in accuracy, this same workflow could be applied to gather morphology data from imaged melt pools. It is often desired to measure the width and height of melt pools in AM parts to gain insight into the thermal history during manufacturing, and the Mask R-CNN model used here to measure the cell size also has the potential to produce accurate results for melt pool size and shape if trained to do so. A melt pool analysis tool such as this could also be paired with the melt pool generation tool introduced here to aid in replicating observed melt pool structures for simulation. However, it is often difficult to distinguish the entire melt pool profile from SEM images of prepped samples, making the segmentation of melt pools likely more difficult than the segmentation of cells.

The melt pool structure generation tool introduced here has been developed to an adequate level to be applied to other FEA simulations. This tool should be paired with simulation methods presented in previous studies to test for improvements in accuracy due to improved melt-pool geometry and to further investigate FGMs. It would also be very interesting, although complex, to create a melt pool structure generation tool such as this for three dimensional structures capable of creating rotated scanning directions.

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