A micromechanical-based computational framework for modeling the mechanical properties of the metallic parts fabricated by selective laser melting

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A Thesis

Entitled

A Micromechanical-based Computational Framework for Modeling the Mechanical Properties of the Metallic Parts Fabricated by Selective Laser Melting

By

Arman Ahmadi

Submitted to the Graduate Faculty as partial fulfillment of the requirements for the Master of Science Degree in Mechanical Engineering

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May 2016
In recent years, a type of additive manufacturing (AM) called selective laser melting (SLM) has attracted significant attention for the manufacturing of metallic materials. SLM is a process by which a laser beam locally melts powder particles and forms a melting pool in order to generate complex and net-shaped parts that are useful in various industries. These pools solidify and join the neighboring pools as the laser beam moves forward to create the processed part. The solidified pools are connected to each other by a thin surface that has different material properties than the bulk material. Defects and voids between the connected pools will form during the manufacturing process, which will have a significant effect on the mechanical properties of the final sample. Depending on the size of each pool and the size of powder, each of the solidified melts pools may contain several grains. In SLM samples, in addition to the grain boundaries, the microstructure has another set of connecting surfaces between the melt pools. Some of the previously reported works on SLM processed materials have studied the microstructure of the manufactured part by optical microscopes, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and X-Ray Diffraction (XRD). However, no studies have yet
measured these properties at the microstructural level to predict the macroscopic mechanical response of the manufactured material.

In this work, a computational framework is developed to model the mechanical response of SLM processed materials by considering both the grain and melt pool in the material. In this model, individual melt pools are approximated as overlapped cylinders, each of which contains several grains. The neighboring melt pools are connected to each other by cohesive surfaces. The proposed computational model can be used to predict the effect of various microstructural properties, including melt pool size, the overlap between neighboring melt pools, texture, process-induced defects, and the orientation of layers with respect to the loading direction, on the mechanical properties of the manufactured sample. 316L stainless steel flat dog bone parts with different values of laser power, scanning velocity, and scanning direction are fabricated in order to study the influence of laser parameters on mechanical properties of the fabricated parts and to relate them to microstructural modeling.

The experimental results indicate that by decreasing scanning velocity or increasing laser power in SLM, the size of the created melt pools, bonding between them, and the density increase which leads to higher mechanical properties. The same results are achieved in finite element simulation of the microstructural modeling by considering the different size of melt pool, porosity, and orientation. The model with bigger size of melt pools has higher tensile strength, which is consistent with the experiments. Furthermore, the model with higher percent of internal porosity and lower density has lower mechanical properties. For the orientation, the FE model shows that applying $\langle 111 \rangle$ crystal orientation in loading direction leads to improving in mechanical properties.
To My Loving Parents
Acknowledgements

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List of Abbreviations

AM .................................. Additive Manufacturing
BCC .................................. Body-Centered Cubic
BD .................................. Building Direction
CZM .................................. Cohesive Zone Model
DCB .......................... Double Cantilever Beam
FCC .......................... Face-Centered Cubic
EDM .......................... Electro Discharge Machine
ENF .......................... End Notch Flexure
LD .......................... Loading Direction
RMSE .......................... Root-Mean-Square Error
RVE .......................... Representative Volume Element
SD .......................... Scanning Direction
SEM .......................... Scanning Electron Microscope
SLM .......................... Selective Laser Melting
TEM .......................... Transmission Electron Microscopy
TSL .......................... Traction-Separation Law
XRD .......................... X-Ray Diffraction
### List of Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>( \gamma^\alpha )</td>
<td>Total shear strain in system ( \alpha )</td>
</tr>
<tr>
<td>( \tau_0 )</td>
<td>Initial yield stress</td>
</tr>
<tr>
<td>( \tau_s )</td>
<td>Saturation stress</td>
</tr>
<tr>
<td>( \sigma^\gamma )</td>
<td>Cauchy stress</td>
</tr>
<tr>
<td>( \mu_\alpha )</td>
<td>Orientation of a slip system ( \alpha ) in the single crystalline</td>
</tr>
<tr>
<td>( \omega^\alpha )</td>
<td>Rotation of the slip system</td>
</tr>
<tr>
<td>( \delta )</td>
<td>Separation</td>
</tr>
<tr>
<td>( \mu )</td>
<td>Viscosity parameter</td>
</tr>
<tr>
<td>( \delta )</td>
<td>Separation</td>
</tr>
<tr>
<td>( \nu )</td>
<td>Poisson ratio</td>
</tr>
<tr>
<td>( C )</td>
<td>Elasticity tensor</td>
</tr>
<tr>
<td>( D )</td>
<td>Degradation variable</td>
</tr>
<tr>
<td>( \bar{D} )</td>
<td>Deformation tensor</td>
</tr>
<tr>
<td>( E )</td>
<td>Stiffness</td>
</tr>
<tr>
<td>( G )</td>
<td>Fracture energy</td>
</tr>
<tr>
<td>( g^\alpha )</td>
<td>Strength of the each slip system</td>
</tr>
<tr>
<td>( H_1 )</td>
<td>Hardening rate of the primary slip system</td>
</tr>
<tr>
<td>( H_2 )</td>
<td>Slip direction for slip system ( \alpha )</td>
</tr>
<tr>
<td>( h_0 )</td>
<td>Initial hardening modulus</td>
</tr>
<tr>
<td>( h_s )</td>
<td>Hardening modulus during stage I deformation</td>
</tr>
<tr>
<td>( h )</td>
<td>Hatch spacing</td>
</tr>
<tr>
<td>( h_{\alpha\beta} )</td>
<td>Hardening moduli matrix</td>
</tr>
<tr>
<td>( I )</td>
<td>Identity tensor</td>
</tr>
<tr>
<td>( K )</td>
<td>Cohesive stiffness</td>
</tr>
<tr>
<td>( K_c )</td>
<td>Fracture toughness</td>
</tr>
<tr>
<td>( L_{ij} )</td>
<td>Tensor of elastic moduli</td>
</tr>
<tr>
<td>( m_{ij}^\alpha )</td>
<td>Slip plane normal for slip system ( \alpha )</td>
</tr>
<tr>
<td>( P )</td>
<td>Laser power</td>
</tr>
<tr>
<td>( q )</td>
<td>Latent/self hardening ratio</td>
</tr>
<tr>
<td>( s_{i}^\alpha )</td>
<td>Slip direction for slip system ( \alpha )</td>
</tr>
</tbody>
</table>
\( t \) .......................... Layer thickness
\( U \) .......................... Displacement
\( v \) .......................... Scanning velocity
\( \dot{\gamma} \) .......................... Jaumann stress
Chapter 1

1. Introduction

This chapter scrutinizes previous studies of the selective laser melting method and the microstructural modeling. Then, the crystal plasticity theory and cohesive zone method, which are implemented in the finite element (FE) model, are studied in detail. Finally, the additive manufacturing method, which is used in the experiments, is explained.

1.1 Background

Selective laser melting (SLM) is an additive manufacturing (AM) technology that uses a 3D CAD model to melt a powder material. A laser follows the CAD file in a layer-by-layer approach to create the desired shape. SLM first started in 1995 at the Fraunhofer Institute in Achen, Germany, resulting in the ILT SLM patent [1], and since then numerous studies have been conducted on SLM of different materials including: aluminum, cobalt, chrome, titanium, nitinol, and stainless steel [2-5]. The following are some of the recent studies related to SLM of stainless steel. In 2004, Morgan et al. [6] studied the density of the fabricated stainless steel in SLM. They found that changing the laser parameters led to a change in density of the specimens. To measure the density of the parts, they applied two
different techniques. First, a measurement involving mass/volume was performed using a digital balance and vernier calipers. Second, they applied a xylene impregnation technique [7], which calculates the density by a series of weight measurements. Yasa et al. [8] in 2011, stated that laser re-melting can improve the surface quality and reduce the porosity of the fabricated 316L stainless steel parts, but the production time also increases. Laser re-melting means re-scanning the same layer of the powder during or after a previous scanning. In 2014, Antony et al. [9] investigated the effect of process parameters such as laser power, scanning velocity, and beam size on the geometrical characteristics and balling phenomenon of 316L stainless steel samples. They asserted that laser power can enhance energy density remarkably resulting in a higher melting temperature and bigger melt pools. Yan et al. [10] studied the manufacturability and performance of lightweight 316L stainless steel lattice structures fabricated by SLM. These lattice structures are manufactured in a wide range of volume fractions at various orientations, which are useful in lightweight structures. They noticed that higher volume fraction of the lattice structures resulted in higher yield strength and Young’s modulus. Shifeng et al. [11] compared the influence of melt pool boundaries on microscopic slipping, ductility, and fracture of the manufactured 316L stainless steel samples fabricated along different directions. They conducted that the pool boundaries have a notable effect on anisotropy and ductility of SLM processed samples. In 2015, Zhao et al. [12] analyzed the chemical elements in melt pool boundaries and studied the phase composition, hardness, stiffness, and tensile properties of SLM processed 420 stainless steel. They proved that melt pool boundaries have a lower hardness and Young’s modulus than other areas of the pool. Furthermore, vertical parts had higher tensile strength compared with the horizontal ones due to the direction of melt pool
In 2016, Miranda et al. [13] studied the effect of SLM processing parameters and building strategies on shear strength, hardness, and density of 316L stainless steel samples using statistical analysis. They presented six models to optimize the properties of the fabricated parts.

In computational material science, the microstructural study is a growing area of interest. By knowing the physical laws that are related to the mesoscale dimension, a model can be produced to extract the macroscopic properties of the material. For modeling a polycrystalline structure, the geometrical properties of the grains must be either obtained experimentally or approximated by Voronoi tessellation method. One of the recent studies in this area is related to the work of Simonovski et al. [14] which evaluated the effect of grain orientations on surface cracks of the 316L stainless steel. Their model includes 212 randomly oriented grains. They proved that the maximum crack tip opening displacements is related to the stiffness of the grains. In 2011 [15], they provided a computational framework for FE simulation of intergranular crack growth in a polycrystalline aggregate. They used cohesive zone model (CZM) to study the damage in grains boundaries. CZM illustrates the separation which happens across an extended crack. In 2013 [16], they studied the influence of grain boundary strength and cohesive parameters on the macroscopic response of a stainless steel polycrystalline aggregate. They applied cohesive elements for the interaction of grain boundaries. In 2015 [17], they provided a model to study the initiation and evolution of intergranular cracking in polycrystalline 304 stainless steel. They applied cohesive surfaces for the grain boundaries and found that these have significantly lower numerical convergence issues than when using cohesive elements.
They also explained that including shear damage initiation leads to a faster damage evolution and decrease in the material’s ductility.

There are several studies of FE modeling of SLM processed materials that predict their properties. For instance, in 2004, Kolossov et al. [18] proposed an FE model for SLM of titanium to determine the effect of melting on the temperature field of the fabricated part. They found that the evolution of thermal conductivity plays a crucial role in properties of the material. In 2009, Dong et al. [19] proposed a transient 3D FE model to study the phase transformation during the SLM process. They established a linear dependence relation between the laser power and the maximum temperature on the surface of the powder. In 2013, Hussein et al. [20] developed an FE model to predict the dimension of the melt pool at different scanning velocities, temperatures, and stress fields in 316L stainless steel layers fabricated on the powder bed in SLM. Their FE model demonstrated that the length of the melt pool increases at a higher scanning velocity, but that the depth and width of the pool decreases. In 2014, Papadakis et al. [21] suggested a methodical model reduction for an FE simulation of large components with suitable computational time to analyze thermo-mechanical effects in SLM processed IN718 parts. This model was used to fabricate high-quality components. In 2015, Li [22] conducted an experimental and numerical simulation of the constitutive behavior of stainless steel struts and microlattices processed by SLM. He found that the tensile and compressive stress are localized at two ends of a strut member of a microlattice, which then determines the separation mode in a fracture. In 2016, Huang et al. [23] introduced an FE model to simulate the SLM of TiAl6V4 to study the effect of energy density, volume shrinkage, and hatch distance on the temperature distribution of the process. They asserted that increased laser power has a greater effect on thermal
performance than the reduced scan velocity, which can enhance melt pool dimensions. In addition, a smaller hatch distance and time interval reduce the temperature gradient, improve the wetting condition, and increase the density of the samples. Foroozmehr et al. [24] suggested a 3D FE model to simulate the melt pool size during laser melting of 316L stainless steel. They found that the size of a melt pool changes from the first track to the next, but it gains a stable condition after a few tracks. There are no research studies on measuring the properties at the microstructural level and connecting them to the macroscopic mechanical response of the manufactured material in SLM.

In this work, a computational framework is developed to model the mechanical response of 316L stainless steel samples processed by SLM by considering both the grains and melt pools. Melt pools are approximated as overlapped cylinders which are connected to each other by CZM. Then, the effect of various microstructural properties is investigated, including melt pool size, the overlap between neighboring melt pools, texture, process-induced defects, and the orientation of layers with respect to the loading direction, on the mechanical properties of the manufactured sample. For experimental verification, some specimens are fabricated with different values of laser power, scanning velocity, and scanning direction using SLM. Tensile tests and SEM tests are performed on the fabricated parts to obtain the mechanical and microstructural properties, respectively.

1.2 Crystal Plasticity Theory

Crystal plasticity can be used for relating the plastic behavior of the crystalline materials to their microstructures. It is useful for modeling crack propagation, fatigue,
creep, texture design, fracture criteria, etc. In this section, a review of plasticity theory, the constitutive law, and the related subroutine for single crystals are studied.

1.2.1 Plastic Flow in Metals

There are some fundamental theories of monocristalline plasticity in single crystal modeling. First, Taylor [25] in 1932 claimed that for accommodating an arbitrary strain increment on a crystal, five independent slip systems are needed. Schmid [26] proposed a law for the occurrence of slip due to applied load on a single crystal. Asaro [27] expressed a planar double slip model and studied the nonuniform and localized deformation in a single crystal. Peirce et al. [28] proposed detailed numerical simulations of single crystal by considering their localization behavior. Then, 3D simulation of crystalline structures including multi-slip structures like face-centered cubic (FCC) and body-centered cubic (BCC) was investigated [29, 30].

In metals, plastic deformation starts when dislocations move in a particular crystallographic direction. Actually, slip occurs where the resolved shear stress is high and acting along a specific crystallographic direction. Several slip systems can be activated in larger deformations because of lattice rotations and hardening on activated planes. Some of the major slip systems in different crystal structures are mentioned below:
- FCC: twelve slip systems of the type of (1 1 1)[1 1 0]
- BCC: forty-eight slip systems, twelve of the type of (1 1 0)[1 1 1], twelve of the type of (1 1 2)[1 1 1], and twenty-four of the type of (1 2 3)[1 1 1].
- Hexagonal Close-Packed (HCP): Three slip system of (0 0 0 1)[1 1 1 0]
1.2.2 Constitutive Law

In crystal plasticity theory, the plastic shear strain $\gamma$ is considered as dislocation flow on a slip system. Shear strains are represented in tensor format. The detailed mathematical theory was offered by Hill [31], Rice [32], and Asaro [33, 34]. The following is a simple summary of this theory.

The total strain rate of an elastic-plastic crystal during loading is the sum of elastic strain rate and plastic strain rate. So the time derivative of the displacement can be written as:

$$\frac{\partial \mathbf{u}_i}{\partial x_j} = \dot{\mathbf{u}}_j^{el} + \dot{\mathbf{u}}_j^{pl} \quad (1.1)$$

Plastic strain rate is related to the slipping rate of the $\alpha$-th slip system by summing over all the activated systems.

$$\dot{\mathbf{u}}_j^{pl} = \sum_{\alpha} \dot{\gamma}_s^\alpha \mathbf{s}_i^\alpha m_j^\alpha \quad (1.2)$$

where $\mathbf{s}_i^\alpha$ specifies the slip direction for slip system $\alpha$ and $m_j^\alpha$ the slip plane normal for slip system $\alpha$. Slip system is used for the combination of the slip plane and shear direction. $\dot{\gamma}^\alpha$ is the slipping rate.

By defining the strain tensor $\varepsilon_{ij}$ as

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial \mathbf{u}_i}{\partial x_j} + \frac{\partial \mathbf{u}_j}{\partial x_i} \right) \quad (1.3)$$

The plastic strain rate can be derived by:
\[ \dot{\varepsilon}_{ij}^{pl} = \sum_{\alpha} \frac{\gamma_{ij}^\alpha}{2} (s_{ij}^\alpha m_j^\alpha + s_{ij}^\alpha m_i^\alpha) \]  

(1.4)

The Schmid resolved shear stress on each slip system is defined by:

\[ \tau^\alpha = s_i^\alpha \sigma_j m_j^\alpha \]  

(1.5)

The relation between stress and strain rate of the elastic-plastic monocrystal is given by:

\[ \sigma_{ij} = L_{ijkl} \varepsilon_{kl}^{el} = L_{ijkl} (\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^{pl}) \]  

(1.6)

where \( L_{ijkl} \) is the tensor of elastic moduli.

Peirce [35] stated the plastic slip rate in a slip system in the form of power-law expression. In this equation, \( \gamma_0^\alpha \) is a reference strain rate and \( g^\alpha \) is the the strength of the each slip system.

\[ \dot{\gamma}^\alpha = \gamma_0^\alpha \text{sgn}(\tau^\alpha) \left| \frac{\tau^\alpha}{g^\alpha} \right|^n \]  

(1.7)

The evolution of the strength of the slip system \( g^\alpha \) is represented by:

\[ \dot{g}^\alpha = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^\beta \]  

(1.8)

where \( h_{\alpha\beta} \) is the hardening moduli matrix. In the formula, \( \alpha = \beta \) is used for self-hardening and \( \alpha \neq \beta \) for latent hardening. There are some important hardening models that a few of them are discussed below.

An isotropic hardening modulus is proposed by Taylor [25] for single crystals holding \( h \) constant for all the slip systems. This shows the crystal hardens isotropically but is not able to verify the higher latent hardening rates.
Modification to Taylor’s model is proposed by Nakad and Keh [36] that can be used for higher latent hardening rate.

\[ d\tau \alpha = H_1 \sum_i d\gamma_i + H_2 \sum_m d\gamma_m \]  

(1.9)

where \( H_1 \) is the hardening rate of the primary slip system and \( H_2 \) is the hardening rate of other slip system.

Havner and Shalaby [37] represented the anisotropic hardening of a single crystal. Because of the relative rotation of crystalline material, all the slip systems have equal hardening.

Peirce et al. [28] proposed a modified model of hardening with lower hardening and is more in agreement with experimental results. For self-hardening, they proposed a hyperbolic secant function in which self-hardening starts with higher value and then disappears after getting the saturation of the resolved shear stress.

\[ h_{\tau \alpha} = h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right) \]  

(1.10)

\[ h_{\tau \beta} = q h(\gamma) : \alpha \neq \beta \]

Where the initial hardening modulus is shown by \( h_0 \), initial yield stress \( \tau_0 \), saturation stress \( \tau_s \), and latent/self hardening ratio \( q \).

Bassani and Wu [38, 39] recommended a different method for the hardening modulus to explain the three stages of hardening in crystalline materials.
\[ h_{\alpha\alpha} = \left( (h_0 - h_s) \sech^2 \left( \frac{(h_0 - h_s) \gamma_\alpha}{\tau_s - \tau_0} \right) + h_s \right) G(\gamma^\beta; \beta \neq \alpha) \]
\[ h_{\alpha\beta} = q h_{\alpha\alpha} \quad : \alpha \neq \beta \]
\[ G(\gamma^\beta; \beta \neq \alpha) = 1 + \sum_{\beta \neq \alpha} f_{\alpha\beta} \tanh \left( \frac{\gamma^\beta}{\gamma_0} \right) \]

where \( h_0 \) stands for the initial hardening modulus, \( h_s \) the hardening modulus during stage I deformation, \( \tau_0 \) the initial yield stress, \( \tau_s \) the saturation stress, \( \gamma^\alpha \) the total shear strain in system \( \alpha \), \( \gamma^\beta \) the total shear strain in system \( \beta \), and \( f_{\alpha\beta} \) the interaction strength between slip systems.

The hardening moduli saturate after gaining the resolved shear stress \( \tau_s \) because of the hyperbolic secant function which starts to decrease as the total shear strain increases, and the resolved shear stress reaches its peak value to \( \tau_s \). Then, \( h_s \) determines a finite hardening rate for each slip system. The function \( G \) has a role on cross-hardening that happens between slip systems during stage II hardening.

### 1.2.3 Numerical Implementation

An ABAQUS user subroutine is proposed for single crystals by Huang [40] that can be used for FCC and BCC materials. This subroutine is applicable for small deformation theory and the theory of finite-strain and finite-rotation. The current strength \( g^\alpha \), normal to slip plane \( m^\alpha \), slip direction \( s^\alpha \), shear strain \( \gamma^\alpha \), and resolved shear stress \( \tau^\alpha \) are the parameters with solution state variables. This subroutine updates the values of stresses and the solution dependent state variable to the values that are calculated at the end.
of the increment. The subroutine has the possibility of using either the Newton-Rhapson iterative method to solve nonlinear incremental equations or the linearized solution method. The summary of the formulation is explained below.

Jaumann rate of Cauchy stress $\sigma^Y$ which is a stress rate on the axes that rotate with the crystal lattice is equal to:

$$\sigma^Y = \underline{C} : \underline{D} - \sigma(I : \underline{D}) - \sum_{\alpha} \gamma^\alpha Y_\alpha \quad (1.12)$$

Such that $\underline{C}$ is the elasticity tensor, $I$ is the identity tensor, $\underline{D}$ is deformation tensor, $\underline{C} : \underline{D}$ is the tensor scalar product, and $Y_\alpha$ is the Jaumann stress which is given below:

$$Y_\alpha = \underline{C} : \mu_\alpha + \underline{\omega}_\alpha, \sigma - \sigma \cdot \underline{\omega}_\alpha \quad (1.13)$$

$\mu_\alpha$ represents the orientation of a slip system $\alpha$ in the single crystalline, $\omega_\alpha$ is the rotation of the slip system due to the rotation of crystal lattice, and $\omega_\alpha, \sigma$ is a tensor product.

To determine the increment of plastic strain in a slip system, the tangential rate method is applied which considers the change in shear strain rates over the time. This increment of plastic strain is given as:

$$\Delta \gamma'_\alpha = [(1 - \Theta)\gamma'_\alpha + \Theta \gamma'_{r + \alpha}] \Delta t \quad (1.14)$$

where the integration constant is shown by $\Theta$ which ranges from 0 to 1 depending on the implicit/explicit method. Then the Taylor expansion of the slipping rate is expressed
by:

\[
\dot{\gamma}_a^{i+\Delta t} = \dot{\gamma}_a^i + \frac{\partial \dot{\gamma}_a^i}{\partial \tau^a} \Delta \tau^a + \frac{\partial \dot{\gamma}_a^i}{\partial g^a} \Delta g^a
\]

(1.15)

Here \( \Delta \tau^a \) is the increment of resolved shear stress and \( \Delta g^a \) is the current strength in slip system. Therefore, the incremental relation for plastic strain in slip system is proposed by substituting the equation (1.15) to (1.14) as follows:

\[
\Delta \gamma_a = [\dot{\gamma}_a^i + \Theta \frac{\partial \dot{\gamma}_a^i}{\partial \tau^a} \Delta \tau^a + \Theta \frac{\partial \dot{\gamma}_a^i}{\partial g^a} \Delta g^a] \Delta t
\]

(1.16)

For the hardening equation, the increments of resolved shear stress \( \Delta \tau^a \) are related to the strain increments \( \Delta \varepsilon_{ij} \) as follows:

\[
\Delta \tau^a = (L_{ijkl} \mu_{kl} + \omega_{ik} \sigma_{j} + \omega_{jk} \sigma_{ik})[\Delta \varepsilon_{ij} - \sum_{\beta} \mu_{ij}^\beta \Delta \gamma_{ij}^\beta]
\]

(1.17)

In addition, Huang [40] proposed the corotational stress increments as:

\[
\Delta \sigma_{ij} = (L_{ijkl} \Delta \varepsilon_{kl} - \sigma_{ij} \Delta \varepsilon_{kk}) - \sum_{\alpha} [L_{ijkl} \mu_{kl} + \omega_{ik} \sigma_{j} + \omega_{jk} \sigma_{ik}] \Delta \gamma_{ij}^\alpha
\]

(1.18)

Finally, by the following linear algebraic equation that is derived using the equations (1.8) and (1.17) in equation (1.16), the increments of the shear strain in the slip systems for any strain increments \( \Delta \varepsilon_{ij} \) can be achieved.

\[
\sum \left[ \delta_{ij} + \Theta \Delta t \frac{\partial \dot{\gamma}_{ij}}{\partial \tau^a} L_{ijkl} \mu_{kl} + \omega_{ik} \sigma_{j} + \omega_{jk} \sigma_{ik} \right] \mu_{ij}^\beta - \Theta \Delta t \frac{\partial \dot{\gamma}_{ij}}{\partial \tau^a} h_{ij} \text{sign}(\dot{\gamma}_{ij}^i) \Delta \gamma_{ij}^\beta = \dot{\gamma}_{ij}^i \Delta t + \Theta \Delta t \frac{\partial \dot{\gamma}_{ij}}{\partial \tau^a} L_{ijkl} \mu_{kl} + \omega_{ik} \sigma_{j} + \omega_{jk} \sigma_{ik} \Delta \varepsilon_{ij}
\]

(1.19)
1.3 Cohesive Zone Modeling

The cohesive zone model (CZM) represents a gradual phenomenon during which separation happens across an extended crack or cohesive zone that is restricted by cohesive tractions [41]. It can be used to model fracture metals, ceramic materials, composites, adhesively bonded polymers, grain interfaces, etc. [42-44]. Figure 1-1 shows the CZM for interfacial separation.

![Cohesive Zone Model](image)

Figure 1-1: Cohesive zone model for interfacial separation [45].

In CZM, the separation between the surfaces happens when the damage exceeds a limitation within a cohesive zone.

1.3.1 Various CZM

The response of the CZM is evaluated by the definition of the traction-separation law (TSL). This law can be expressed by considering two of three main parameters, cohesive strength $\sigma_c$ (a maximum surface traction in which damage initiates), critical displacement $\delta_c$ (the amount of separation in which the interface completely fails), and cohesive energy $G_c$ (the area under traction-separation curve). There are several traction-
separation models that can be used as the fracture model. Some common types of these models are exponential, polynomial, trapezoidal, bilinear, trilinear, parabolic, etc.

**Exponential model:** Xu and Needleman [46] suggested the polynomial and exponential traction-separation law to simulate the particle debonding in metal matrices. The exponential model is shown in Figure 1-2.

![Exponential traction-separation model](image)

The interface potential for the exponential CZM is defined by:

$$\phi(\Delta_n, \Delta_t) = \phi_n + \phi_n \exp\left(-\frac{\Delta_n}{\delta_n}\right) \left\{ [1-r+\frac{\Delta_n}{\delta_n}]1-q-\frac{r-q}{r-1}\frac{\Delta_n}{\delta_n}\right\} \exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)$$

$$q = \frac{\phi}{\phi_n}, r = \frac{\Delta_n}{\delta_n}$$

where $\phi_n$ is the work of the normal separation, $\phi_t$ the work of tangential separation, $\Delta_n$ and $\Delta_t$ are the normal and tangential displacement respectively, $\delta_n$ and $\delta_t$ are the corresponding characteristic length, and $\Delta_n^*$ is the value of $\Delta_n$ after complete shear separation with $T_n=0$. 

14
According to this potential function, the cohesive surface tractions are obtained by:

\[
T_n = \frac{\partial \phi}{\partial \Delta_n} = -\frac{\phi_n}{\delta_n} \exp\left(-\frac{\Delta_n}{\delta_n}\right) \left[\frac{\Delta_n}{\delta_n} \exp\left(-\frac{\Delta_n^2}{\delta_n^2}\right) + \frac{1}{r-1} \left(1 - \exp\left(-\frac{\Delta_n^2}{\delta_n^2}\right)\right)\right] \quad (1.21)
\]

\[
T_t = \frac{\partial \phi}{\partial \Delta_t} = -\frac{\phi_t}{\delta_t} \left(2 \frac{\Delta_t}{\delta_t}\right) \exp\left(-\frac{\Delta_n}{\delta_n}\right) \exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)
\]

The work of normal and tangential separation which are the area under their traction-separation curve, is derived by:

\[
\phi_n = \exp(1)\sigma_c \delta_n
\]

\[
\phi_t = \sqrt{\frac{\exp(1)}{2}} \tau_c \delta_t
\]

**Trapezoidal model:** This model is suggested by Tvergaard and Hutchinson [47] to study the crack growth resistance in elastic-plastic material. It is appropriate for ductile material. This model is shown in Figure 1-3.

![Trapezoidal traction-separation model](image)

Figure 1-3: Trapezoidal traction-separation model

In this model, a non-dimensional effective separation parameter is defined by:
\[ \delta = \sqrt{\left(\frac{\delta_n^c}{\delta_n}\right)^2 + \left(\frac{\delta_t^c}{\delta_t}\right)^2} \]  

(1.23)

Such that $\delta_n^c$ and $\delta_t^c$ are the critical values of normal and tangential separation respectively.

By defining the interface potential as:

\[ \phi(\Delta_n, \Delta_t) = \Delta_n^c \int_0^\delta \sigma(\delta')d\delta' \]  

(1.24)

Then, the normal and tangential cohesive surface tractions are given below:

\[ T_n = \frac{\partial \phi}{\partial \Delta_n} = \frac{\sigma(\delta)}{\delta} \delta_n \]

\[ T_t = \frac{\partial \phi}{\partial \Delta_t} = \frac{\sigma(\delta)}{\delta} \delta_t \frac{\Delta_n^c}{\Delta_t^c} \]  

(1.25)

The work of separation which is the area under traction-separation curve is represented by;

\[ \phi_0 = 0.5\sigma_c(\delta_c + \delta_2 - \delta_1) \]  

(1.26)

Scheider [48, 49] improved this trapezoidal law by suggesting a model that the initial stiffness of the cohesive zone can be varied, and the curve can be continuously differentiable to reduce the numerical problem (Figure 1-4)
The normal and tangential cohesive surface tractions are given by the following:

\[\begin{align*}
\delta &\leq \delta_c \\
T_n &= \frac{1}{\delta_c} \frac{\delta_n}{\delta_n^c}\sigma_c = \frac{1}{\delta_c \delta_n^c} \sigma_c \\
T_t &= \frac{1}{\delta_t^c} \frac{\delta_t}{\delta_t^c} \sigma_c
\end{align*}\] (1.27)
\[ \delta \geq \delta_c \]
\[ T_n = \frac{\delta_n}{\delta_n^c} \left( 1 - \frac{\delta}{\delta_c^c} \right) \sigma_c \]
\[ T_t = \frac{\delta_t}{\delta_t^c} \left( 1 - \frac{\delta}{\delta_c^c} \right) \sigma_c \]

Such that a non-dimensional effective separation parameter is defined by:

\[ \delta = \sqrt{\left( \frac{\delta_n}{\delta_n^c} \right)^2 + \left( \frac{\delta_t}{\delta_t^c} \right)^2} \]

Then, the work of separation is equal to:

\[ \phi_0 = 0.5 \sigma_c \delta_c \]

Another linear cohesive fracture model is employed by Camacho and Ortiz [44] to simulate the impact damage in brittle materials (Figure 1-6).

Figure 1-6: Camacho linear traction-separation model

### 1.3.2 Cohesive Parameters

As mentioned earlier, for any shape of TSL curves, the cohesive parameters need
to be determined. There are some important parameters in CZM that could be determined from an experiment as an estimation and then optimized by numerical simulation. The following explanations are related to the bilinear traction-separation model (Figure 1-7).

\[ \begin{bmatrix}
    t_n \\
    t_s \\
    t_t
\end{bmatrix} = 
\begin{bmatrix}
    K_{nn} & 0 & 0 \\
    0 & K_{ss} & 0 \\
    0 & 0 & K_{tt}
\end{bmatrix}
\begin{bmatrix}
    \delta_n \\
    \delta_s \\
    \delta_t
\end{bmatrix} \quad (1.31)

Figure 1-7: Bilinear traction-separation model

In this model, TSL is assumed to be linear before damage initiation. The relation between cohesive strength and the separation can be written as:

\[ T_n, T_s, T_t \]

where \( n \) indicates the normal direction and \( s \) and \( t \) are the two orthogonal shear directions. \( K \) represents the cohesive stiffness. As the equation (1.31) shows, it is possible to have both coupled/uncoupled for normal/tangential stiffness components according to the application.

**Damage initiation:** Damage initiation refers to the beginning of degradation of the material interface. Several damage initiation criteria can be used as a function of traction...
or separation. If the damage initiates when the maximum contact stress ratio (or maximum separation ratio) reaches a value of one, it is called maximum stress criterion (or maximum separation criterion).

\[
\max \left\{ \frac{t_n}{t_n^0}, \frac{t_s}{t_s^0}, \frac{t_t}{t_t^0} \right\} = 1
\]  

(1.32)

\[
\max \left\{ \frac{\delta_n}{\delta_n^0}, \frac{\delta_s}{\delta_s^0}, \frac{\delta_t}{\delta_t^0} \right\} = 1
\]  

(1.33)

Quadratic stress criterion (or quadratic separation criterion) supposes that damage starts when the quadratic interaction function below satisfies the value of one.

\[
\left\{ \frac{t_n}{t_n^0} \right\}^2 + \left\{ \frac{t_s}{t_s^0} \right\}^2 + \left\{ \frac{t_t}{t_t^0} \right\}^2 = 1
\]  

(1.34)

\[
\left\{ \frac{\delta_n}{\delta_n^0} \right\}^2 + \left\{ \frac{\delta_s}{\delta_s^0} \right\}^2 + \left\{ \frac{\delta_t}{\delta_t^0} \right\}^2 = 1
\]  

(1.35)

**Damage evolution:** Damage evolution describes the degradation rate of cohesive stiffness when the damage initiation is started. The scalar variable D is used to show the current degradation of the material, and it has the value of zero before the damage initiation and has the value of one when the separation happens. The traction vector is affected by the damage according to:

\[
t = (1 - D)\bar{t}
\]  

(1.36)

such that \(\bar{t}\) is the contact traction without damage at the material interface. By defining an effective separation, the evolution of damage can be described by a combination of normal and tangential separations.
\[ \delta_m = \sqrt{\delta_n^2 + \delta_s^2 + \delta_t^2} \]  

(1.37)

A linear or an exponential softening law for damage evolution based on effective separation is the common method that can be followed in FE software. The linear damage evolution is described below:

\[ D = \frac{\delta_m^f (\delta_m^{\text{max}} - \delta_m^0)}{\delta_m^{\text{max}} (\delta_m^f - \delta_m^0)} \]  

(1.38)

such that \( \delta_m^0 \) is the effective separation at damage initiation, \( \delta_m^f \) is the effective separation at complete failure, and \( \delta_m^{\text{max}} \) is the maximum value of effective separation during the loading history.

The exponential softening in Figure 1-8 is a non-dimensional parameter for the rate of damage evolution.

![Figure 1-8: Traction-separation model with exponential damage evolution](image-url)
Damage evolution can also be defined based on the dissipation of the energy during the process which called fracture energy \( (G) \) and it is equal to the area under traction-separation curve. By defining \( G_T = G_n + G_s + G_t \), the mode-mix definition that is the proportions of the normal and tangential separations at a contact point is as follows:

\[
m_1 = \frac{G_n}{G_T}, \quad m_2 = \frac{G_s}{G_T}, \quad m_3 = \frac{G_t}{G_T}
\]  

(1.40)

According to the equation (1.40), just two of these parameters are independent. Then, based on the power law form of evolution, failure under the mix-mode condition is governed by:

\[
G^c = \left( \left( \frac{m_1}{G_n^c} \right)^\alpha + \left( \frac{m_2}{G_s^c} \right)^\alpha + \left( \frac{m_3}{G_t^c} \right)^\alpha \right)^{-1/\alpha}
\]  

(1.41)

Another criterion for damage evolution is employed by Benzeggagh and Kenane (BK) [52] that is useful when the fracture energies along the tangential directions are the same \( (G_s^c = G_t^c) \).

\[
G^c = G_n^c + (G_s^c - G_n^c) \left( \frac{G_s^c + G_t^c}{G_n^c + G_s^c + G_t^c} \right)^\eta
\]  

(1.42)

such that \( \eta \) is the BK cohesive property parameter.

**Viscous regularization**: One of the difficulties in working with CZM with different initiation and evolution laws in FE software is the numerical convergence problem. An
elastic snap-back instability that happens at the beginning of the damage, results in reducing of the convergence in the Newton-Raphson method [53]. There are some techniques such as viscous regularization to overcome these difficulties. Viscous regularization makes the tangent stiffness of the softening material to be positive for a small time increment. This regularization process includes the viscous stiffness degradation variable $D_v$ that is specified below:

\[ \dot{D}_v = \frac{D - D_v}{\mu} \]  

(1.43)

such that $D$ is the degradation variable measured in the inviscid backbone model and $\mu$ is the viscosity parameter showing the relaxation time of the viscous system. Therefore, in equation (1.36), $D_v$ can be substituted for $D$.

### 1.4 Selective Laser Melting

Additive Manufacturing (AM) is a technology that can be used to synthesize 3D parts. Generally, AM is a process which creates the parts directly from CAD model by adding material in successive layers. This technology was developed in the mid 1980’s [54]. Stereolithography was the first AM method related to polymer technologies and developed in 1984 [55]. There are several AM processes and the differences between them are related to the deposition of the layers and the types of the materials. Fuses deposition modeling (FDM), digital light processing (DLP), electron beam melting (EBM), direct metal laser sintering (DLMS), selective laser sintering (SLS), and selective laser melting (SLM) are some of these technologies.
SLM is a powder-bed AM technique that started in 1995 in Germany, resulting in the basic patent [1]. In this process, a 3D CAD model is used as an input and powder material is deposited into layers with the usual thickness of 20-100 µm by a blade or a roller. Each layer has specific information of the related geometry, parameters, physical supports, and the scanning trajectory. Then, laser beam locally melts the powder in each layer of deposition, and this process continues layer by layer until the 3D build is complete. This fabrication carries out inside a chamber with controllable amounts of argon or nitrogen gas at oxygen level of below 500 ppm according to the application. Figure 1-9 shows the schematic SLM of a NiTi scaffold.

![Diagram of SLM process](image)

Figure 1-9: SLM of a metallic model [56].

SLM is able to generate complex three-dimensional metal parts such as stainless steel and nitinol parts that can be used in aerospace, orthopedic, and dental implants. It is especially useful for patient-specific implants which have a complicated shape as well as for the porous structures which prevent stress shielding due to lower stiffness and enable bone to grow within the replacement implant [57-59]. In addition, the ability to fabricate the net shape components reduces the weight that could be useful in some applications. It can also manufacture the fully dense parts without using infiltration, hot isostatic, and
sintering as a post processing. Disadvantages of SLM are related to high cost of this process and long build times for just small size of the parts [60].

1.5 Objectives

The first objective of this work is to evaluate the effect of laser parameters on mechanical properties of 316L stainless steel samples using SLM. The second objective of this work is to propose a computational model to predict the effect of various microstructural properties including the grain size, melt pool size, the overlap between neighbor melt pools, texture, process-induced defects, and the orientation of layers with respect to the loading direction, on the mechanical properties of the manufactured samples. Actually, measuring microstructural properties at the microstructural level and connecting them to the macroscopic mechanical response of the manufactured material.
Chapter 2

2. Methodology of Modeling and Fabrication

In this chapter, an FE simulation is proposed to model the mechanical response of SLM processed 316L stainless steel. The polycrystalline aggregate method, material properties, boundary conditions, and meshes are explained. Then, the experimental procedure for fabrication of stainless steel parts with different values of laser power, scan velocity, and fabrication directions are described.

2.1 Microstructural Modeling

There are numerous computational studies to examine the microstructures in a material. Intergranular stress-corrosion cracking [61-63], heterogeneity of local stresses and strains because of microstructural properties [64], and intrinsic variability in crack tip loading [14, 65] are some of the examples.

By knowing the physical laws that are related at the mesoscale dimension, a model can be produced to extract the correct macroscopic properties of the material. This model is called representative volume element (RVE) that helps us to study the effect of changes in mesoscopic properties on macroscopic ones of a material which can be used for material
optimization. The size of the model is crucial because the effect of local microstructural features averages, should be the same as macroscopic response of the similar material. In addition, considering high level of details for the model, results in remarkable challenging preparation for FE modeling and computationally numerical problems.

In order to model a polycrystalline structure, the geometrical properties of the grains must be obtained. Experimentally, it can be done by using X-ray microscopy [66], 3D X-ray diffraction microscopy [67], and X-ray diffraction contrast tomography [68, 69] which are complicated processes and an extensive and expensive post-processing need to be utilized. Therefore, an approximation of the microstructure in polycrystalline materials can be represented similarly enough to the real structure to have a meaningful analysis of the microstructure. One common way to this goal is implementing Voronoi Tessellation.

This thesis proposes a conventional microstructural model for studying polycrystalline materials created by Voronoi tessellation with different numbers of melt pools and orientations of the grains to incorporate the effect of connecting melt pools beside the grain boundaries in SLM. Individual melt pools can be approximated as overlapped cylinders or spheres, each of them containing several grains and grain boundaries, which are modeled by the cohesive zone method. Crystal plasticity is also applied to account for slip in the grains.

2.1.1 Voronoi Tessellation Method

Voronoi tessellation is an acceptable method to simulate polycrystalline aggregates as it supplies a realistic approximation of the real microstructure of non-uniform grain shapes [70-72]. A set of randomly Poisson points (generators) create the Voronoi cells that
each of them is the set of all points which distances from the related generator are smaller than their distances from the other generators. Recently, some FE models have been employed to simulate polycrystalline gran structures for micromechanical studies based on Voronoi tessellation [73, 74].

A Voronoi tessellation model (Figure 2-1) is used to simulate 316L stainless steel polycrystalline structure and then create different size of the melt pools on it according to SLM process to predict the effect of various microstructural properties (the grain size, melt pool size, the overlap between neighbor melt pools, texture, process-induced defects, and the orientation of layers with respect to the loading direction). This structure is 800 × 200 × 40 µm and contains a total of 100 grains. The selected dimension results in a mean grain size of 40 µm that is consistent with the optical micrograph of this kind of steel in SLM [75, 76].

![Figure 2-1: Voronoi tessellation model with 100 grains.](image)

### 2.1.2 Finite Element Modeling

In SLM samples, in addition to the grain boundaries, the microstructure has another set of connecting surfaces between the melt pools. A computational framework can be
developed to model the mechanical response of SLM processed materials by considering both the grain boundaries and melt pool boundaries in the material. The neighbor melt pools are connected to each other by cohesive surfaces. In Figure 2-2-a), the melt pool that is created because of laser scanning in SLM is shown and b), shows the borders of melt pools connected to each other (dashed lines) where each of these pools contains several grains inside, which are connected to each other through grain boundaries. The FE models in this work are simulated based on these shapes in SLM.

Figure 2-2: a) The melt pool created in SLM of aluminum [77], b) Pole figure of melt pools containing grains in SLM of an aluminum alloy [78].

First of all, three FE models in different sizes and numbers of melt pools are created according to the effects of fabrication parameters on microstructures in ABAQUS (Figure 2-3).
Figure 2-3: Models with different numbers of pools and 100 grains by scanning direction in z, a) 10 pools, b) 19 pools, c) 47 pools.

These models are based on scanning direction (SD) in z and building direction (BD) in y during the fabrication, while the loading is applied in the x direction in FE modeling.

Actually, the front view of the figure 2-4 is shown in figure 2-3.
Figure 2-4: Schematic views of fabricated parts with SD in z, BD in y, and LD in x.

To mesh the model, linear solid tetrahedral elements (C3D4) are applied. 135’067, 86’566, and 187’456 are used for 10 pools, 19 pools, and 47 pools models respectively. The boundary conditions are applied by defining the displacement of the specific nodes of the model. The nodes at the left face of the model are fixed in the x-direction. Two edges of the left face are fixed in a way that they can only move parallel to their edge as shown in Figure 2-5. These boundary conditions prevent rigid body motion of the model [79, 80]. The displacement load is applied to induce the stresses in the model by having all the nodes in the right face move at a strain rate of 3.3e-4 s\(^{-1}\) in x-direction.

Figure 2-5: Illustration of the boundary conditions applied to the model.

For the material properties, anisotropic elasticity and crystal plasticity for 316L
stainless steel are used. The elastic constants of this steel are $C_{ii}=163,680$ MPa, $C_{ij}=110,160$ MPa, and $C_{jj}=100,960$ MPa [81]. The parameters for crystal plasticity are optimized by curve fitting of macroscopic response of polycrystalline aggregate to tensile test data for the material that considers hardening modulus $h_0=75$ MPa, stage I stress $\tau_s=75$ MPa, initial yield stress $\tau_0=150$ MPa, and Taylor’s hardening $q=1$ [81]. These material properties are implemented into the FE software ABAQUS by a user subroutine [40].

Melt pools boundaries are modeled using cohesive zone model (CZM), and the grains boundaries are assumed to be perfect, which is a valid assumption because experiments have shown that pools boundaries are remarkably weaker compared to the grains boundaries and defects usually initiate between these pool boundaries. Shifeng et al. [11] argued that the melt pool boundaries have the unstable nonmetallic elements such as C, O, and Si that decrease near these boundaries which worsen the mechanical properties of pool boundaries in comparison with grain boundaries. A simplification assumption is made to consider the same material properties to all pool boundaries. In this work, cohesive surface (CS) with damage initiation and evolution are applied in FE modeling. For the model containing 19 melt pools, the stiffness of the pool boundaries are taken as: $K_{nn}=200e6$ MPa, $K_{ss}=K_n=\frac{K_{nn}}{2(1+\nu)}=77e6$ MPa. For damage initiation, the quadratic traction criterion is used (equation 1-34) with $t_n^0=550$ MPa and based on the assumption of $\delta_n^0=\delta_s^0=\delta_t^0$ [16], both shear tractions are selected as $t_s^0=t_t^0=210$ MPa. For damage evolution, the fracture energy of $G=10$ MPa with linear softening is used [15] (The method
for the calibration of these parameters is explained in chapter 4).

Convergence issues are one of the prominent concerns in working with CZM. By defining a small viscosity in CZM, the numerical problems could be solved considerably. In this work, $\mu = 3.3$ is selected which is less than 10% of time step ($T = 303$ s) [80] to avoid having large effect on maximum traction, cohesive energy, and final results. In addition, to increase the convergence of the model, cohesive surface with node to surface discretization and small sliding contact formulation [17] are used for the interactions of the pool boundaries.

During fabrication, changing the laser parameters have a notable effect on the density of the fabricated parts. Increasing the scan speed or decreasing the laser power, leads to lower energy density and higher porosity that affect the mechanical properties. To evaluate the effect of internal porosity that happens during fabrication, three different percentages of porosity (0.77%, 1.0%, and 1.5%) [8] are created on the model with 19 melt pools. The shape and the position of the porosity are assumed in circular and elliptical cross-sections and scattered randomly along the scanning direction (Figure 2-6).
Figure 2-6: Models with different percent of porosity, a) 0.77% porosity, b) 1.0% porosity, c) 1.5% porosity

2.1.3 Crystal Orientation

In this work, the effect of the texture on the response of the FE model is studied. Two types of crystal orientations are utilized in the grains. First, a random orientation is allocated to each grain in order to model the untextured material. Second, the textured orientation is applied to each grain such that the <111> directions of the lattice is distributed along the axial direction (the x direction in figure 2-3) based on Gaussian distribution and the <001> directions are scattered randomly [82].
2.2 Fabrication

In this section, the method of fabrication, manufacturing parameters, material characteristics, and mechanical tests which are used in the experiment are brought.

2.2.1 Phenix Systems PXM

In this study, the fabrication of all samples is conducted by using a SLM machine PXM Phenix/3D systems (Figure 2-7). This machine has the maximum laser power of 300 W, and it is equipped with a Ytterbium fiber laser with the laser wavelength of 1070 nm and beam quality of \( M^2 < 1.2 \). The profile of the beam is Gaussian (TEM00), and its diameter is approximately 80 \( \mu \)m. The machine contains a metal scraper and roller to create the powder layers. The feeding piston inside the machine moves the powder upward and then the scraper stacks up the powder from the feeding piston and the roller deposits it on the platform. Afterwards, the laser melts the powder according to the geometry and defined parameters. When the melted powder is solidified, the piston moves downward and the roller brings the next layer, and this process is repeated till the desired part is fabricated. During fabrication, argon is purged to avoid oxidation of the surface of the parts.
2.2.2 Process Parameters and material

The fabrication is conducted using an austenite AISI 316L stainless steel in the form of metallic powder. This type of steel has anti-corrosion property because of molybdenum addition. The composition of this steel is shown in Table 2-1.

Table 2.1 Composition of 316L stainless steel powder

<table>
<thead>
<tr>
<th></th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>Mn</th>
<th>Si</th>
<th>N</th>
<th>P</th>
<th>C</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wt%</td>
<td>16.5-18.5</td>
<td>10-13</td>
<td>2-2.5</td>
<td>2 max</td>
<td>1 max</td>
<td>0.1 max</td>
<td>0.04 max</td>
<td>0.03 max</td>
<td>0.02 max</td>
</tr>
</tbody>
</table>

In fabricating dense parts from stainless steel powder, the optimized process parameters are provided by Phenix Company. To study the effect of laser parameters in SLM on mechanical properties of the parts, other tests are completed by changing laser power, scanning velocity, and laser direction. Table 2-2 shows the optimal parameters achieved by Phenix Company for 316L stainless steel parts.
Table 2.2 Process Parameters used in manufacturing 316l stainless steel parts

<table>
<thead>
<tr>
<th>Laser power (Watt)</th>
<th>Scanning velocity (mm/s)</th>
<th>Hatch distance (µm)</th>
<th>Layer thickness (µm)</th>
<th>Energy input (J/mm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>129</td>
<td>1400</td>
<td>50</td>
<td>30</td>
<td>61.43</td>
</tr>
</tbody>
</table>

The energy input is obtained by:

$$E = \frac{P}{vht}$$

Such that $P$ stands for laser power, $v$ scanning velocity, $h$ hatch spacing, and $t$ layer thickness [84].

2.2.3 Experimental Procedure

In order to study the effect of laser parameters in SLM on mechanical properties of the 316L stainless steel parts and to relate them to microstructural modeling, various laser powers, scanning velocities, and fabrication directions are tried.

Various scanning strategies can be followed during fabrication. As Figure 2-8 shows, in the unidirectional method, the laser always starts from the same side of the parts, while in bidirectional scanning, the laser moves across the surface in a zigzag pattern. In the third method, the laser moves with bidirectional vectors in one direction for the first layer and then moves with bidirectional vectors in transverse direction for the second layer, and this procedure continues during fabrication (cross-hatching technique).
First, one series (each series contains 3 parts) of flat dog bone samples (Figure 2-9 with the thickness of 2 mm) is fabricated with the scanning direction similar to method “c” in Figure 2-8 and the fabrication parameters that were mentioned earlier (P = 0.43P_{\text{max}} = 129 \text{ W}, v = 1400 \text{ mm/s}).
Second, the rest of the parts are fabricated with unidirectional method according to method “a” in transverse direction of the parts (Figure 2-8) and with different values of laser powers and scanning velocities as presented in Table 2-3:

Table 2.3 Laser parameters used for fabrication of the parts.

<table>
<thead>
<tr>
<th>Steps</th>
<th>Laser power (W)</th>
<th>Scanning velocity (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>129</td>
<td>1400</td>
</tr>
<tr>
<td>2</td>
<td>144</td>
<td>1400</td>
</tr>
<tr>
<td>3</td>
<td>159</td>
<td>1400</td>
</tr>
<tr>
<td>4</td>
<td>174</td>
<td>1400</td>
</tr>
<tr>
<td>5</td>
<td>129</td>
<td>1540</td>
</tr>
<tr>
<td>6</td>
<td>129</td>
<td>1680</td>
</tr>
</tbody>
</table>

2.3 Mechanical tests

The fabricated parts are separated from the platform surface by using an electro discharge machine (EDM) which is a method to remove samples by recurring current discharges between two electrodes (Figure 2-10).
Tensile tests are conducted by MTS 810 Material Test System (Figure 2-11) with the maximum load of 100 kN on all of the non-standard flat dog bone samples. The tests are carried out with the strain rate of $3.3\times10^{-4} \text{ s}^{-1}$ (cross speed of 0.5 mm/min) based on ASTM/E8 standard [86]. Each tensile test is obtained from an average of the three experiments.
Chapter 3

3. Results: Evolution and Discussion

In this chapter, the results of calibrating the CZM in an FE model, the effect of laser parameters in the experimental studies, and the effect of microstructural properties on the mechanical properties of the fabricated samples are discussed.

3.1 Model Calibration

The crucial parameters of the CZM include cohesive strength, fracture energy, and initial stiffness. The fracture energy in CZM can be extracted from experiments, but there is no standard method to determine the cohesive strength and initial stiffness, so they usually are obtained by matching the simulation results to the experimental ones [88-90].

The initial stiffness $K$ in CZM should be selected so that $K \gg E/L$ when $E$ is the Young’s modulus of the material and $L$ is the dimension of the specimen [91, 92]. Consequently, the presence of CZM interface will not affect the stiffness of the overall structure. On the other hand, large values of initial cohesive stiffness may cause some numerical difficulties like artificial oscillation of the tractions [93, 94]. According to these
points and considering the stiffness of the 316L stainless steel which is about $E=200'000$ MPa, the initial cohesive stiffness is selected as $K=1000E=200e6$ MPa.

Then, the cohesive strength $t_n^0 = 550$ MPa is chosen by trial and error, based on the best fit achieved during simulation from the range of $(1-4)\sigma_y$ [92]. Actually, in this model, the cohesive strength is almost equal to $t_n^0 \approx 2.5\sigma_y$.

The fracture energy can be obtained by a double cantilever beam (DCB) test or an end notch flexure (ENF) test (Three and four point bend) [45, 90]. For conducting these tests, a pre-crack or notch needs to be made in the specimen. Because of the shape and method of fabrication in our sample, another method is used to estimate the value of cohesive energy. As a reasonable estimation, the fracture energy can be calculated by [46, 95]:

$$G = \frac{K_{lc}^2(1-\nu^2)}{E}$$ (3.1)

Where $K_{lc}$ (MPa.m$^{0.5}$) is fracture toughness, $\nu$ Poisson ratio, and $E$ (MPa) stiffness of the material. 316L stainless steel has the fracture toughness of about 100 MPa.m$^{0.5}$. Based on this formula and trial and error for curve fitting, $G=10$ MPa is achieved as a cohesive property of the model.

By using these parameters for the cohesive surfaces of the model with 19 melt pools and applying curve fitting with experimental results of the part fabricated by $P=129$ (W) and $v=1540$ (mm/s), a reasonable match between numerical modeling and experiment is achieved as shown in Figure 3-1.
Figure 3-1: Comparison of stress-strain curve from experimental measurement and from simulation prediction using CZM.

Strong correlations with low root-mean-square error (RMSE) are observed between the FE prediction and the experimental measurement (RMSE=8.34). The RMSE is a measure of the differences between values predicted by the simulation and the values actually observed in the experiment. In addition, R-squared (a statistical measure of how close the data are to the fitted regression line) for this calibration is $R^2 = %98.22$, which shows a reasonable match between the FE model and the experimental data.

### 3.2 Model Validation

In this section, the results of the changes in fabrication parameters on mechanical properties of the samples are studied.
3.2.1 Effect of Scanning Speed on Mechanical Properties

In order to investigate the effect of scanning velocity on the mechanical properties of the fabricated parts, three different laser speeds of 1400, 1540, and 1680 mm/s are tried, while the other parameters of the laser are kept constant (P= 129 W and h= 50µm). Figure 3-2 shows that the mechanical properties of the samples decrease as the velocity increases.

![Figure 3-2: Comparison of stress-strain curves with different values of scanning velocities from experimental measurements](image)

Laser power, scanning velocity, and hatch spacing are among the most influential parameters in SLM, and the relation of them to the energy released to the scanning area known as energy density (J/mm³) can be shown as below [84, 96]:

\[ E = \frac{P}{vht} \]  \hspace{1cm} (3.2)

Where P is the laser power (W), v is the scanning velocity (mm/s), h is the hatch distance (mm), and t is the layer thickness (mm). By decreasing scanning velocity, the
energy density of the laser increases which results in full melting because of more particle fusion [97]. When the energy density increases, it causes to have bigger melt pools and lower porosity that enhance the density of the fabricated parts. Clearly, the material with lower porosity has higher mechanical properties. In addition, the binding between melt pools improves by reducing scanning velocity [98, 99]. Figure 3-3 shows the effect of scanning velocity on the porosity of the fabricated stainless steel parts according to Li’s work [100].

![Figure 3-3: The porosity variation in different speed velocities (mm/s), a) v= 90, b) v= 120, c) v= 150, d) v= 180 [100].](image)

The values of yield stress, ultimate stress, and elongation for the parts fabricated by laser power of 129 W and different scanning velocities are mentioned in Table 3-1.
Table 3.1 Tensile tests results for samples with different scanning velocities.

<table>
<thead>
<tr>
<th>Laser power (W)</th>
<th>Scanning velocity (mm/s)</th>
<th>Yield stress (MPa)</th>
<th>Ultimate stress (MPa)</th>
<th>Elongation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>129</td>
<td>1400</td>
<td>265</td>
<td>280</td>
<td>0.68</td>
</tr>
<tr>
<td>129</td>
<td>1540</td>
<td>218</td>
<td>232</td>
<td>0.65</td>
</tr>
<tr>
<td>129</td>
<td>1680</td>
<td>173</td>
<td>181</td>
<td>0.58</td>
</tr>
</tbody>
</table>

Furthermore, by increasing scanning velocity, the balling effect, which is an unfavorable defect associated with SLM, happens due to worsening wetting ability during the process. It occurs when the underlying substrate is not wetted by the molten material because of the surface tension which causes the liquid to spheroidise [101]. This balling phenomenon has a negative effect on surface roughness and mechanical properties of the part [102]. In Figure 3-4, the balling effect on the part with scanning velocity of 1680 mm/s is shown.

![Image of balling effect](image_url)
3.2.2 Effect of Laser Power on Mechanical Properties

In order to study the effect of laser power on the mechanical properties of the fabricated parts, four different laser powers of 129, 144, 159, and 189 (W) are tried while the other parameters of the laser are kept constant (v= 1400 mm/s and h= 50µm). Figure 3-5 shows that the mechanical properties of the samples increase as the power increases.

![Stress-strain curves with different laser power](image)

**Figure 3-5:** Comparison of stress-strain curves with different values of laser power from experimental measurements

Similar to decreasing in scanning velocity, by increasing laser power, the energy density of the laser increases according to equation (3.1) which results in full melting because of increased particle fusion [97]. When the energy density increases, it causes to have bigger melt pools and lower porosity that increase the density of the fabricated parts. Clearly, the material with lower porosity has higher mechanical properties. In addition, by increasing laser power, the scan tracks become continuous, the balling initiation is reduced, wetting and spreading of the molten pools are improved which eventuate to higher
mechanical properties of the part [102]. On the other hand, furrowing and discoloring are some disadvantages of increasing laser power due to creating deep melt pools and overheating of the process. It is worth noting that although these defects have a harmful effect on surface quality of the fabricated parts, because of strong bonding of each furrow to its neighbors, they do not make noticeable reduction in mechanical properties [98].

It is worth mentioning that laser power has much higher impact on mechanical properties in comparison with the scanning velocity. Especially, there is an immense effect on the strain and toughness of the fabricated parts in a way that by increasing power from 129 W to 189 W, the strain and toughness increase more than 15 times which is considerable. Zhao et al. [103] explained that by increasing laser power, the proportion of α phase (Fe-Cr) in 420 stainless steel decreased and the phase austenite (CrFe7C0.45) increased which result in higher mechanical properties. Antony et al. [9] also studied the effect of SLM on chemical composition of the fabricated parts. They showed that by increasing laser power, the percent of chromium and nickel rises too that leads to higher strength and toughness. Cr has a remarkable effect on the toughness and nickel on the toughness and strength of the stainless steel [104]. Table 3-2 summarizes the values of yield stress, ultimate stress, and elongation for the parts fabricated with the scanning velocity of 1400 mm/s and different laser powers.

Table 3.2 Tensile tests results for samples with different laser powers.

<table>
<thead>
<tr>
<th>Laser power (W)</th>
<th>Scanning velocity (mm/s)</th>
<th>Yield stress (MPa)</th>
<th>Ultimate stress (MPa)</th>
<th>Elongation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>129</td>
<td>1400</td>
<td>265</td>
<td>280</td>
<td>0.68</td>
</tr>
</tbody>
</table>
3.2.3 Effect of Scanning Direction on Mechanical Properties

To study the effect of scanning direction on the mechanical properties of the fabricated parts, two different scanning methods are evaluated (Unidirectional and cross-hatching with zigzag scanning). Figure 3-6 shows that the mechanical properties of the samples increase in cross-hatching technique of the laser.

![Stress-strain curve comparison](image)

Figure 3-6: Comparison of stress-strain curves with different scanning strategy from experimental measurements

Morgan et al [105] investigated that cross-hatching technique reduces the porosity of the fabricated part significantly in comparison with the unidirectional method that can
be explained for increasing of tensile strength and toughness of the material. Thijs et al [106] also governed the same results for Ti-6Al-4V. They stated that besides having more isotropic structure in cross-hatching strategy, the density of the part is ameliorated, and the pores are more spheroidized ones that are less detrimental to mechanical properties. Table 3-3 compares the mechanical properties of the parts fabricated with two scanning methods.

Table 3.3 Tensile tests results for samples with different scanning directions.

<table>
<thead>
<tr>
<th>Scanning strategy</th>
<th>Yield stress (MPa)</th>
<th>Ultimate stress (MPa)</th>
<th>Elongation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unidirectional</td>
<td>265</td>
<td>280</td>
<td>0.68</td>
</tr>
<tr>
<td>Cross-hatching</td>
<td>350</td>
<td>394</td>
<td>2.62</td>
</tr>
</tbody>
</table>

### 3.3 Simulation studies

In this section, the results of the numerical simulation based on the effect of the laser parameters on microstructure of the SLM fabricated parts are studied.

#### 3.3.1 Effect of Melt Pools Size on Microstructures

As mentioned earlier, the bigger melt pools are created in SLM by increasing the laser power or decreasing the scanning velocity that leads to higher mechanical properties [98, 99]. In order to show this behavior, three models with different number and size of melt pools (10, 19, and 47 pools) are constructed, and they are assumed to be related to scanning velocities of 1400, 1540, and 1680 mm/s respectively. Earlier, the model containing 19 pools was calibrated with the stress-strain curve of the part fabricated with 1540 mm/s scanning velocity. Now, the part with higher scanning velocity (1680 mm/s) is
simulated with the model by lower number and bigger size of pools (10 Pools) and the part with lower scanning velocity (1400 mm/s) is simulated with the model by higher number and smaller size of pools (47 Pools). This is just an assumption that is made to show the trend of experimental results, so the dimension of the pools may not be the same as the real condition (Figure 2-2).

As shown in Figure 3-7, by increasing the number of pools (smaller pool size in constant volume), the decline in mechanical properties can be seen.

![Figure 3-7: Comparison of stress-strain curves with different numbers of melt pools from simulation](image)

Based on this result, as the size of melt pools in the model increases (lower numbers of melt pool in constant volume), tensile properties in the simulation increase too. It is in accordance with the experimental results about the effect of laser parameters on the size of melt pools. Thanks to this consequence, a computational model can be proposed to find the
optimum configuration of microstructural properties in SLM. In Table 3-4, the RMSE and the R-squared error are shown for these calibrations.

Table 3.4 RMSE and R-squared errors related to calibrations of the FE models with the experiments.

<table>
<thead>
<tr>
<th>FE model</th>
<th>Experiment</th>
<th>RMSE</th>
<th>% R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 melt pools</td>
<td>v=1400 mm/s (P=129 W, h=50 µm)</td>
<td>24.79</td>
<td>88.10</td>
</tr>
<tr>
<td>19 melt pools</td>
<td>v=1540 mm/s (P=129 W, h=50 µm)</td>
<td>8.34</td>
<td>98.22</td>
</tr>
<tr>
<td>47 melt pools</td>
<td>v=1680 mm/s (P=129 W, h=50 µm)</td>
<td>15.10</td>
<td>90.10</td>
</tr>
</tbody>
</table>

3.3.2 Effect of Porosity on Microstructures

According to the literature, higher porosity which decreases the mechanical properties is the result of increasing the scanning velocity or decreasing the laser power [98, 99]. To evaluate the effect of porosity on the microstructure, three different percent of porosity (0.77%, 1%, and 1.5%) are created on the model with 19 melt pools as shown in figure 2-5. As Figure 3-8 shows, by increasing this defect on the FE model, the value of ultimate stress decreases which is consistent with the experiment.
3.3.3 Effect of Crystal Orientation on Microstructures

In order to study the effect of texture on the simulation, two types of random and textured orientation are implemented in the model with 19 melt pools. Figure 3-9 shows that the model with textured orientation has higher mechanical properties.
It is worth noting that by doing some post-processing on the fabricated parts in SLM such as cold working and making desired texture on the material, the mechanical properties can be improved [107, 108]. In addition, a strong <001> texture is created along the building direction during SLM because of the variation of the thermal gradient and the growth rate [109]. Actually, the moving heat source builds elongated melt pools that have an influence on the directionality of the solidification, so the columnar grains grow from the melt pools boundaries toward the center of the melt pool [78].
Chapter 4

4. Conclusions and Future Work

The major contributions of this study are summarized below. In addition, some suggestions are presented that can be followed as valuable research topics for future studies.

4.1 Conclusions

In this work, a conventional microstructural model for studying polycrystalline materials is proposed to predict the effect of various microstructural properties including the melt pool size, texture, process-induced defects, and the orientation of layers on the mechanical properties of the manufactured 316L stainless steel samples in SLM. In this model, individual melt pools are approximated as overlapped cylinders, each of which contains several grains. These pool boundaries are modeled by the CZM. To connect the effect of fabrication parameters (laser power and scanning velocity) on microstructural properties of the fabricated samples, three FE models of different sizes and pool numbers are simulated. In addition, various levels of porosity in one of the models are applied to investigate the influence of internal porosity on the mechanical properties of processed
samples. Crystal orientation has a crucial influence on the tensile response of an FE model. To study this effect, stress-strain curves of two models with random and texture orientations are compared.

To study the effect of manufacturing parameters on the tensile properties of the fabricated parts via SLM, several specimens are fabricated with different values of laser power and scanning velocity. Then, the effect of changes in these parameters on microstructural properties is connected to the FE models. Additionally, the influence of scanning strategy on mechanical properties of the processed parts is evaluated by comparing two scanning methods (unidirectional and cross-hatching).

It is shown that by decreasing scanning velocity or increasing laser power in SLM, the energy density increases, which leads to lower porosity, higher density, bigger melt pools, stronger bonding between them and, finally, higher mechanical properties. Additionally, balling phenomenon, which is a detrimental defect in SLM, occurs as the scanning velocity increases or laser power decreases because of worsening wetting ability during the process. The balling defect has a harmful influence on surface roughness and mechanical properties of the part. On the other hand, furrowing and discoloring are unfavorable circumstances of increasing laser power due to creating deep melt pools and overheating of the process. These defects have a negative impact on the surface quality of the fabricated parts. It is worth noting that laser power has a much higher effect on mechanical properties in comparison with the scanning velocity because of changes in percent of chromium and nickel at higher values of laser power. The tensile tests also show that the samples fabricated by cross-hatching technique have higher mechanical properties than the ones fabricated by unidirectional scanning strategy. According to the literature,
unidirectional method manufactures the part with higher porosity, which leads to lower tensile properties.

To connect the properties of the material at the microstructural level to the macroscopic mechanical response of the manufactured sample, the cohesive properties of the model containing 19 melt pools are calibrated with the tensile properties of the parts fabricated by P=129 W and v=1540 mm/s. Based on FE results, as the size of melt pools in the model increases, tensile properties in the simulation increase as well. This is consistent with the experimental results of the effect of laser parameters on the size of melt pools. Furthermore, similar to experimental results, the FE model with higher percent of porosity shows lower mechanical properties. Finally, the FE model with texture orientation shows higher tensile strength in comparison to the model by random orientation, which highlights the effect of fabrication direction and post processing on crystal orientations and mechanical properties of the fabricated part.

These achievements pave the way for fabrication of more productive parts by SLM and enhance a particular macroscopic mechanical property by considering microscopic modeling. The proposed computational model can also be used to find the optimum configuration of microstructural properties. This model can predict whether the pool boundaries or the grain boundaries are the major site in the failure and fracture of the material.
4.2 Suggestions for Future Work

This work can be continued in different aspects. Below are some of the suggestions to make this thesis more practical.

- The effect of other parameters in SLM on mechanical properties like hatch distance, laser diameter, purged gas during fabrication, different scanning methods, pre-heating of the powder before fabrication, etc. can be studied in an experiment and also relating the effect of these parameters such as hatch distance in FE modeling by changing overlapping of the pools.

- In FE modeling, there is an essential step in selecting an appropriate boundary condition. Applying real boundary conditions on the RVE leads to closer material properties in the microstructural phenomenon to macrostructural behavior in a global sense [110]. One of the most common and effective boundary conditions is periodic boundary condition (PBC) [111, 112] which resembles the model in real size. For applying PBC, the model should have periodic mesh. To make this study more realistic, PBC can be utilized.

- In this model, due to some difficulties in implementation and numerical problems, the cohesive properties are just considered for pool boundaries and grain boundaries are assumed to be perfect. In the next work, the cohesive element of the surface can be defined for grain boundaries as well to make the model more practical and develop the properties of both grain and pool boundaries.

- By relating laser parameters to the microstructural configuration, an optimized model of microstructural properties can be employed in order to enhance a particular macroscopic mechanical property and then connecting the microstructural properties to the
macroscopic mechanical response of the manufactured material. In this way, the optimized parameters in SLM of the desired material can be extracted by the computational model instead of doing the trial and error in experiments which is costly, time-consuming, and imprecise.
References


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